Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:04 AM EDT

PDB ID	:	4RCR
Title	:	STRUCTURE OF THE REACTION CENTER FROM RHODOBACTER SPHAEROIDES R-26 AND 2.4.1: PROTEIN-COFACTOR (BACTERIOCHLOROPHYLL, BACTERIOPHEOPHYTIN, AND CAROTENOID) INTERACTIONS
Authors	:	Komiya, H.; Yeates, T.O.; Chirino, A.J.; Rees, D.C.; Allen, J.P.; Feher, G.
Deposited on	:	1991-09-09
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

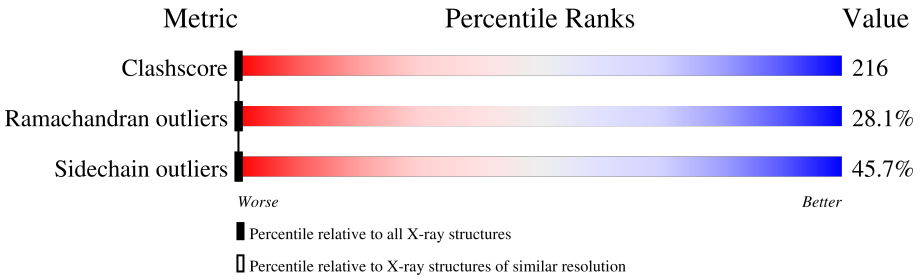
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	281	5% 32% 38% 21% 5%
2	M	307	5% 36% 34% 21% .
3	H	260	5% 28% 36% 23% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	L	283	-	-	X	-
4	BCL	M	310	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	M	311	-	-	X	-
5	BPH	L	284	-	-	X	-
5	BPH	M	312	-	-	X	-
6	U10	L	285	-	-	X	-
6	U10	M	313	-	-	X	-
7	BOG	M	308	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6764 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	266	2120	1433	336	343	8	0	0	0

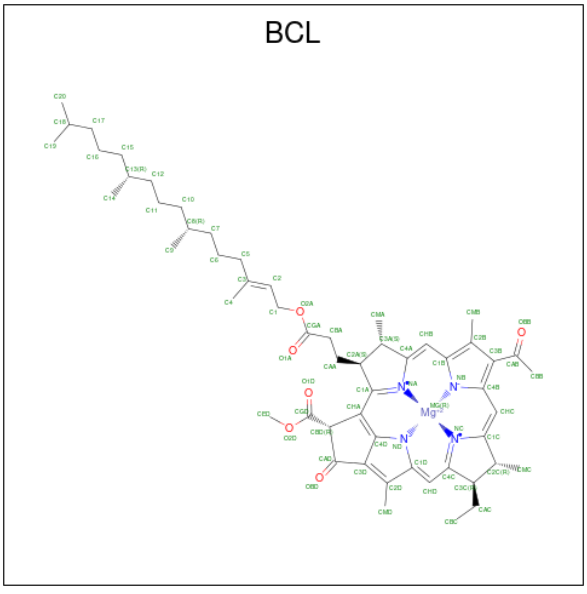
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	296	2361	1579	386	386	10	0	0	0

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

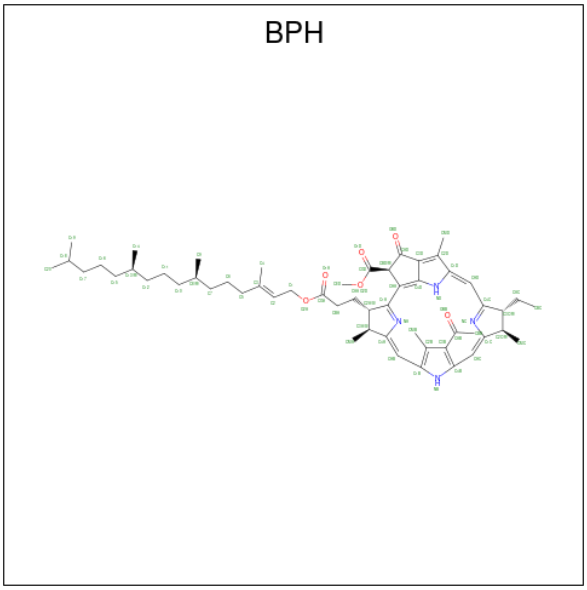
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	237	1806	1156	310	331	9	0	0	0

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



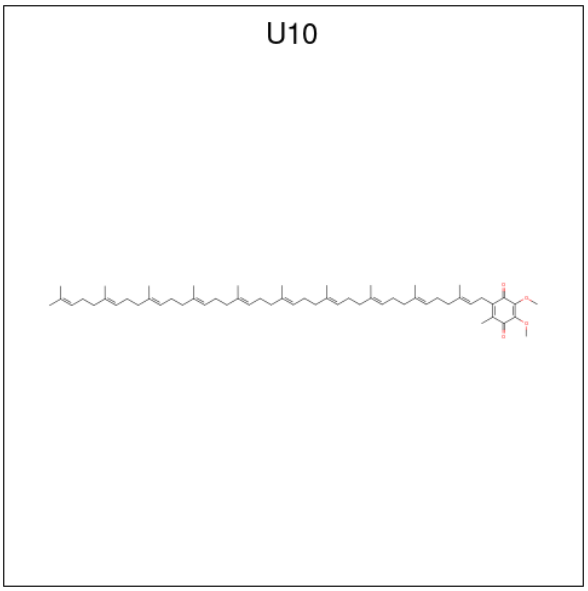
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



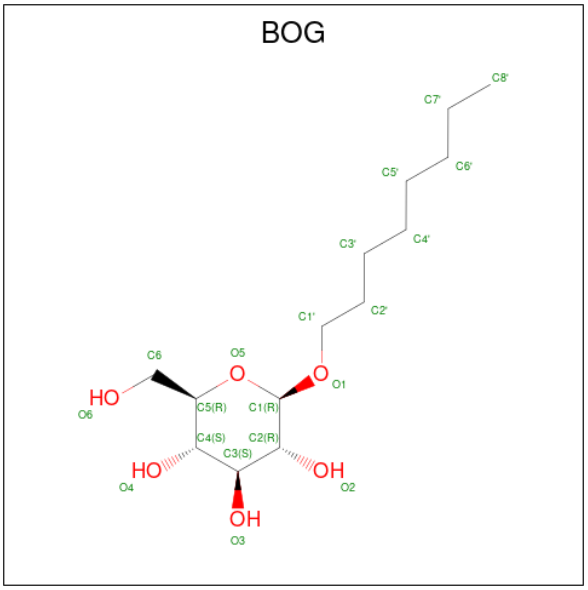
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 41 37 4	0	0
6	M	1	Total C O 51 47 4	0	0

- Molecule 7 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total C O 20 14 6	0	0

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Fe 1 1	0	0

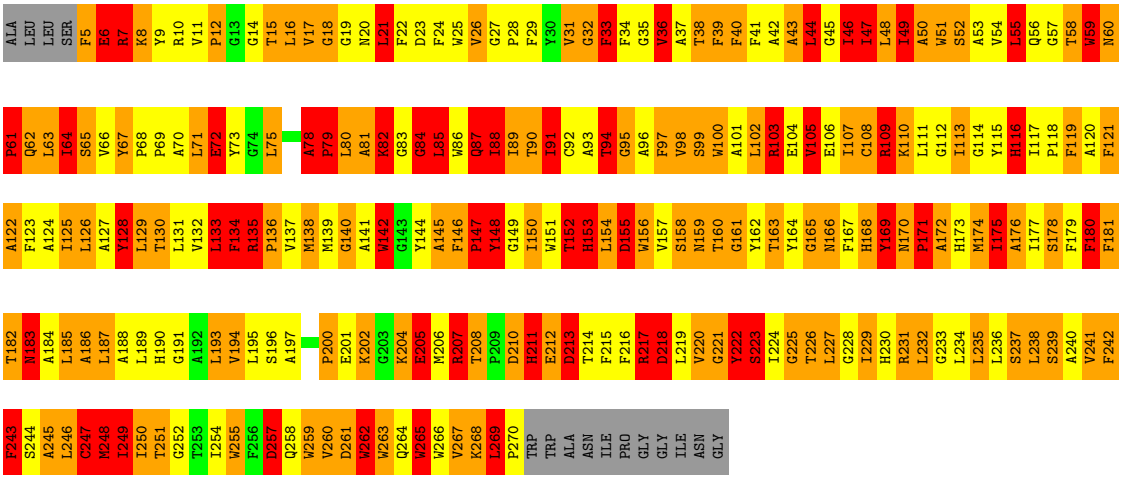
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

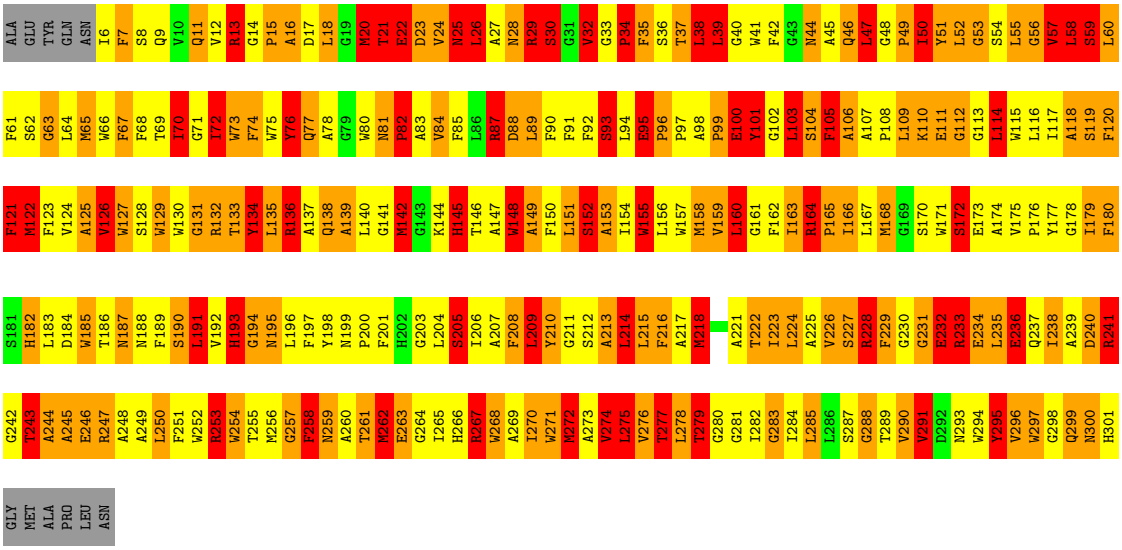
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain L: 5% 32% 38% 21% 5%



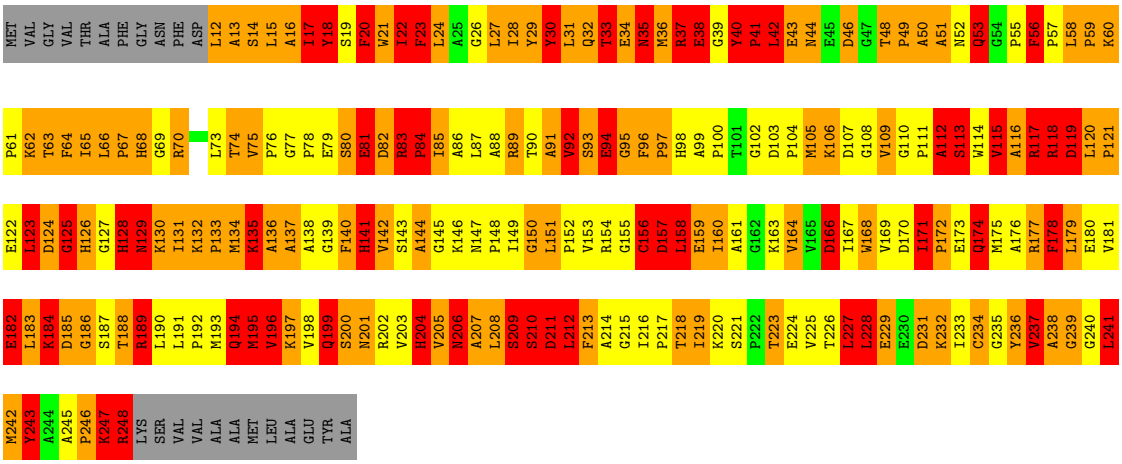
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER

Chain M: 5% 36% 34% 21%



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER

Chain H: 5% 28% 36% 23% 9%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.227 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, BPH, U10, BOG, BCL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	L	1.01	1/2203 (0.0%)	1.69	48/3014 (1.6%)
2	M	1.03	0/2452	1.71	52/3348 (1.6%)
3	H	1.16	4/1854 (0.2%)	1.95	48/2523 (1.9%)
All	All	1.06	5/6509 (0.1%)	1.78	148/8885 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	36
2	M	0	29
3	H	2	39
All	All	2	104

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	53	GLN	C-N	17.61	1.64	1.33
3	H	56	PHE	C-N	-12.37	1.10	1.34
3	H	248	ARG	CD-NE	-6.33	1.35	1.46
3	H	248	ARG	NE-CZ	-5.38	1.26	1.33
1	L	94	THR	CA-CB	5.02	1.66	1.53

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	248	ARG	CD-NE-CZ	40.26	179.96	123.60
2	M	13	ARG	NE-CZ-NH1	14.66	127.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	13	ARG	NE-CZ-NH2	-11.69	114.46	120.30
3	H	177	ARG	NE-CZ-NH1	-10.41	115.10	120.30
3	H	248	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	M	247	ARG	NE-CZ-NH1	9.65	125.13	120.30
2	M	30	SER	N-CA-CB	9.51	124.76	110.50
2	M	121	PHE	CB-CA-C	9.44	129.29	110.40
1	L	169	TYR	CB-CG-CD2	-9.15	115.51	121.00
3	H	227	LEU	CB-CA-C	8.94	127.19	110.20
2	M	205	SER	N-CA-CB	8.77	123.65	110.50
1	L	59	TRP	CB-CA-C	8.67	127.74	110.40
3	H	37	ARG	NE-CZ-NH1	8.66	124.63	120.30
3	H	42	LEU	CB-CA-C	8.59	126.52	110.20
1	L	169	TYR	CB-CG-CD1	8.49	126.09	121.00
1	L	211	HIS	CA-CB-CG	-8.26	99.55	113.60
3	H	23	PHE	N-CA-CB	8.25	125.45	110.60
1	L	168	HIS	N-CA-CB	8.15	125.28	110.60
1	L	109	ARG	NE-CZ-NH1	-8.14	116.23	120.30
3	H	238	ALA	CB-CA-C	8.01	122.11	110.10
1	L	135	ARG	NE-CZ-NH1	7.99	124.30	120.30
2	M	285	LEU	CB-CA-C	7.99	125.38	110.20
2	M	148	TRP	CA-CB-CG	7.97	128.84	113.70
2	M	21	THR	CA-CB-CG2	7.96	123.54	112.40
2	M	164	ARG	NE-CZ-NH1	7.92	124.26	120.30
2	M	38	LEU	CB-CA-C	7.78	124.98	110.20
1	L	158	SER	N-CA-CB	7.75	122.13	110.50
3	H	23	PHE	CA-CB-CG	7.71	132.41	113.90
1	L	231	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	L	109	ARG	NE-CZ-NH2	7.67	124.13	120.30
3	H	211	ASP	CB-CA-C	7.65	125.70	110.40
2	M	184	ASP	CB-CG-OD1	-7.64	111.43	118.30
3	H	184	LYS	N-CA-CB	7.60	124.28	110.60
2	M	267	ARG	NE-CZ-NH2	7.49	124.05	120.30
2	M	121	PHE	CA-CB-CG	-7.48	95.94	113.90
2	M	21	THR	N-CA-CB	7.33	124.23	110.30
2	M	241	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	L	217	ARG	NE-CZ-NH1	-7.18	116.71	120.30
3	H	70	ARG	NE-CZ-NH2	7.17	123.89	120.30
3	H	178	PHE	N-CA-CB	7.17	123.50	110.60
1	L	105	VAL	CA-CB-CG1	7.12	121.58	110.90
2	M	236	GLU	N-CA-CB	7.10	123.38	110.60
3	H	22	ILE	CB-CA-C	7.04	125.68	111.60
1	L	205	GLU	CA-CB-CG	6.99	128.77	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	207	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	M	148	TRP	CB-CA-C	6.94	124.28	110.40
1	L	82	LYS	N-CA-CB	6.88	122.98	110.60
2	M	243	THR	N-CA-CB	6.86	123.32	110.30
3	H	35	ASN	CB-CA-C	6.82	124.04	110.40
2	M	134	TYR	CB-CG-CD1	-6.73	116.96	121.00
2	M	155	TRP	CA-CB-CG	6.71	126.44	113.70
1	L	5	PHE	CA-CB-CG	6.69	129.96	113.90
3	H	20	PHE	N-CA-CB	6.67	122.60	110.60
2	M	132	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	M	121	PHE	CB-CG-CD1	-6.62	116.16	120.80
2	M	247	ARG	CD-NE-CZ	6.57	132.80	123.60
1	L	155	ASP	CB-CA-C	6.56	123.53	110.40
3	H	204	HIS	N-CA-CB	6.54	122.37	110.60
1	L	5	PHE	N-CA-CB	6.48	122.26	110.60
3	H	171	ILE	N-CA-CB	6.46	125.65	110.80
2	M	142	MET	N-CA-CB	-6.40	99.08	110.60
1	L	254	ILE	CB-CA-C	6.39	124.37	111.60
1	L	180	PHE	CB-CG-CD1	-6.37	116.34	120.80
1	L	257	ASP	CB-CG-OD1	6.32	123.98	118.30
1	L	163	THR	N-CA-CB	6.32	122.30	110.30
1	L	78	ALA	CB-CA-C	6.28	119.52	110.10
2	M	95	GLU	CA-CB-CG	6.27	127.19	113.40
2	M	277	THR	N-CA-CB	6.25	122.18	110.30
1	L	213	ASP	CB-CG-OD1	6.25	123.92	118.30
1	L	142	TRP	CA-CB-CG	6.24	125.55	113.70
2	M	142	MET	CA-CB-CG	-6.18	102.80	113.30
2	M	218	MET	CG-SD-CE	6.18	110.09	100.20
3	H	33	THR	N-CA-CB	6.17	122.03	110.30
3	H	177	ARG	NE-CZ-NH2	6.16	123.38	120.30
2	M	88	ASP	CB-CA-C	6.15	122.71	110.40
1	L	220	VAL	CB-CA-C	6.08	122.96	111.40
1	L	222	TYR	CB-CG-CD2	-6.07	117.36	121.00
3	H	182	GLU	CG-CD-OE1	6.07	130.44	118.30
2	M	32	VAL	CB-CA-C	6.06	122.92	111.40
2	M	76	TYR	CB-CG-CD1	6.05	124.63	121.00
1	L	246	LEU	CB-CA-C	5.99	121.58	110.20
2	M	76	TYR	CB-CG-CD2	-5.97	117.42	121.00
3	H	204	HIS	N-CA-C	5.97	127.12	111.00
2	M	21	THR	OG1-CB-CG2	5.97	123.73	110.00
3	H	195	MET	CB-CA-C	5.92	122.24	110.40
3	H	212	LEU	CB-CA-C	5.86	121.32	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	142	TRP	N-CA-CB	5.84	121.12	110.60
2	M	236	GLU	OE1-CD-OE2	-5.83	116.30	123.30
3	H	168	TRP	CA-CB-CG	5.83	124.78	113.70
2	M	233	ARG	NE-CZ-NH1	-5.82	117.39	120.30
2	M	121	PHE	CB-CG-CD2	5.81	124.86	120.80
1	L	259	TRP	CA-CB-CG	5.77	124.66	113.70
1	L	36	VAL	CB-CA-C	5.73	122.29	111.40
1	L	116	HIS	N-CA-C	5.71	126.42	111.00
2	M	95	GLU	N-CA-CB	5.71	120.87	110.60
2	M	127	TRP	CB-CA-C	5.69	121.78	110.40
2	M	145	HIS	CB-CA-C	-5.68	99.03	110.40
3	H	43	GLU	N-CA-CB	5.67	120.80	110.60
3	H	177	ARG	N-CA-CB	5.64	120.76	110.60
1	L	130	THR	C-N-CA	5.63	135.76	121.70
3	H	66	LEU	CB-CA-C	5.62	120.89	110.20
1	L	213	ASP	OD1-CG-OD2	-5.60	112.66	123.30
1	L	218	ASP	CB-CG-OD1	-5.59	113.26	118.30
3	H	81	GLU	CA-CB-CG	5.54	125.59	113.40
1	L	105	VAL	CB-CA-C	5.54	121.92	111.40
3	H	248	ARG	NH1-CZ-NH2	-5.52	113.32	119.40
3	H	29	TYR	CB-CG-CD1	-5.52	117.69	121.00
3	H	115	VAL	CB-CA-C	5.51	121.87	111.40
1	L	103	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	L	213	ASP	CA-CB-CG	5.49	125.47	113.40
2	M	70	ILE	CA-CB-CG2	5.49	121.87	110.90
2	M	262	MET	N-CA-CB	5.48	120.46	110.60
1	L	262	TRP	CB-CG-CD2	-5.40	119.58	126.60
2	M	274	VAL	CB-CA-C	5.39	121.63	111.40
2	M	100	GLU	CB-CG-CD	5.38	128.73	114.20
3	H	141	HIS	N-CA-CB	5.38	120.28	110.60
1	L	210	ASP	CB-CA-C	5.36	121.12	110.40
3	H	228	LEU	CB-CA-C	5.34	120.34	110.20
1	L	134	PHE	CB-CG-CD1	-5.34	117.06	120.80
3	H	75	VAL	CB-CA-C	5.31	121.49	111.40
1	L	210	ASP	CB-CG-OD2	5.29	123.06	118.30
3	H	206	ASN	CB-CA-C	5.26	120.92	110.40
2	M	226	VAL	CB-CA-C	5.25	121.39	111.40
3	H	210	SER	O-C-N	5.25	131.10	122.70
2	M	151	LEU	CB-CA-C	5.24	120.16	110.20
1	L	148	TYR	N-CA-CB	5.22	119.99	110.60
1	L	152	THR	CA-CB-CG2	5.21	119.70	112.40
3	H	18	TYR	CB-CG-CD1	-5.20	117.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	182	GLU	CA-CB-CG	5.20	124.84	113.40
3	H	194	GLN	N-CA-CB	5.18	119.92	110.60
3	H	166	ASP	C-N-CA	5.17	134.62	121.70
1	L	48	LEU	CA-CB-CG	5.16	127.17	115.30
3	H	166	ASP	CB-CG-OD2	5.16	122.94	118.30
2	M	89	LEU	CB-CA-C	5.15	119.99	110.20
2	M	272	MET	N-CA-CB	5.14	119.85	110.60
3	H	84	PRO	CA-N-CD	-5.14	104.30	111.50
2	M	295	TYR	CB-CG-CD1	-5.13	117.92	121.00
3	H	37	ARG	CD-NE-CZ	5.12	130.78	123.60
2	M	232	GLU	CG-CD-OE1	-5.12	108.06	118.30
3	H	243	TYR	CA-CB-CG	5.09	123.08	113.40
1	L	152	THR	N-CA-CB	5.08	119.95	110.30
1	L	221	GLY	C-N-CA	5.06	134.36	121.70
1	L	178	SER	N-CA-CB	5.05	118.08	110.50
3	H	208	LEU	N-CA-CB	-5.05	100.30	110.40
3	H	89	ARG	NE-CZ-NH2	5.04	122.82	120.30
2	M	193	HIS	CB-CA-C	5.04	120.47	110.40
2	M	180	PHE	CB-CG-CD1	-5.03	117.28	120.80
3	H	22	ILE	CA-CB-CG2	5.01	120.92	110.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	141	HIS	CA
3	H	204	HIS	CA

All (104) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	112	ALA	Mainchain
3	H	117	ARG	Sidechain
3	H	119	ASP	Mainchain
3	H	120	LEU	Mainchain
3	H	121	PRO	Mainchain
3	H	125	GLY	Mainchain
3	H	128	HIS	Mainchain
3	H	137	ALA	Mainchain
3	H	139	GLY	Mainchain
3	H	140	PHE	Mainchain
3	H	142	VAL	Mainchain
3	H	145	GLY	Mainchain

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Mol	Chain	Res	Type	Group
3	H	150	GLY	Mainchain
3	H	156	CYS	Mainchain
3	H	157	ASP	Mainchain
3	H	159	GLU	Mainchain
3	H	164	VAL	Mainchain
3	H	17	ILE	Mainchain
3	H	174	GLN	Mainchain
3	H	18	TYR	Sidechain
3	H	189	ARG	Sidechain
3	H	199	GLN	Mainchain
3	H	201	ASN	Mainchain
3	H	206	ASN	Mainchain
3	H	209	SER	Mainchain
3	H	218	THR	Mainchain
3	H	22	ILE	Mainchain
3	H	227	LEU	Mainchain
3	H	237	VAL	Mainchain
3	H	241	LEU	Mainchain
3	H	243	TYR	Mainchain
3	H	33	THR	Mainchain
3	H	40	TYR	Mainchain,Sidechain
3	H	41	PRO	Mainchain
3	H	42	LEU	Mainchain
3	H	48	THR	Mainchain
3	H	50	ALA	Mainchain
3	H	96	PHE	Sidechain
1	L	103	ARG	Mainchain
1	L	122	ALA	Mainchain
1	L	142	TRP	Mainchain
1	L	148	TYR	Sidechain
1	L	152	THR	Mainchain
1	L	154	LEU	Mainchain
1	L	155	ASP	Mainchain
1	L	160	THR	Mainchain
1	L	175	ILE	Mainchain
1	L	180	PHE	Sidechain
1	L	181	PHE	Mainchain,Sidechain
1	L	183	ASN	Sidechain
1	L	196	SER	Mainchain
1	L	204	LYS	Mainchain
1	L	211	HIS	Sidechain
1	L	218	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	L	222	TYR	Mainchain,Sidechain
1	L	248	MET	Mainchain
1	L	249	ILE	Mainchain
1	L	255	TRP	Mainchain
1	L	257	ASP	Mainchain
1	L	36	VAL	Mainchain
1	L	44	LEU	Mainchain
1	L	46	ILE	Mainchain
1	L	6	GLU	Mainchain
1	L	61	PRO	Mainchain
1	L	64	ILE	Mainchain
1	L	65	SER	Mainchain
1	L	7	ARG	Sidechain
1	L	75	LEU	Mainchain
1	L	84	GLY	Mainchain
1	L	85	LEU	Mainchain
1	L	88	ILE	Mainchain
1	L	97	PHE	Sidechain
2	M	100	GLU	Mainchain
2	M	13	ARG	Sidechain
2	M	131	GLY	Mainchain
2	M	134	TYR	Sidechain
2	M	136	ARG	Sidechain
2	M	142	MET	Mainchain
2	M	145	HIS	Mainchain
2	M	16	ALA	Mainchain
2	M	193	HIS	Mainchain,Sidechain
2	M	194	GLY	Mainchain
2	M	20	MET	Mainchain
2	M	208	PHE	Sidechain
2	M	21	THR	Mainchain
2	M	210	TYR	Sidechain
2	M	215	LEU	Mainchain
2	M	224	LEU	Mainchain
2	M	228	ARG	Mainchain
2	M	234	GLU	Mainchain
2	M	253	ARG	Mainchain
2	M	254	TRP	Mainchain
2	M	275	LEU	Mainchain
2	M	277	THR	Mainchain
2	M	291	VAL	Mainchain
2	M	30	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	M	50	ILE	Mainchain
2	M	73	TRP	Mainchain
2	M	81	ASN	Mainchain
2	M	87	ARG	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2120	0	2077	1093	0
2	M	2361	0	2279	1145	0
3	H	1806	0	1814	771	0
4	L	117	0	115	116	0
4	M	117	0	113	93	0
5	L	65	0	76	44	0
5	M	65	0	76	47	0
6	L	41	0	52	31	0
6	M	51	0	68	43	0
7	M	20	0	28	7	0
8	M	1	0	0	0	0
All	All	6764	0	6698	2900	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 216.

All (2900) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:73:TRP:CD1	2:M:114:LEU:HG	1.20	1.64
5:M:312:BPH:C11	5:M:312:BPH:C10	1.76	1.61
5:M:312:BPH:C6	5:M:312:BPH:C7	1.78	1.60
1:L:175:ILE:HG21	1:L:243:PHE:CD2	1.24	1.60
2:M:197:PHE:CZ	4:M:310:BCL:HBB2	1.33	1.57
1:L:208:THR:HG23	1:L:211:HIS:CD2	1.41	1.53
2:M:218:MET:HE2	2:M:252:TRP:CZ2	1.46	1.50
2:M:243:THR:CG2	2:M:247:ARG:HE	1.21	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:ILE:HD13	1:L:243:PHE:CE2	1.45	1.47
2:M:35:PHE:HD2	2:M:47:LEU:CD1	1.24	1.46
1:L:269:LEU:HD22	1:L:270:PRO:CD	1.47	1.44
1:L:97:PHE:CE1	4:L:283:BCL:H142	1.51	1.43
5:L:284:BPH:C17	5:L:284:BPH:H143	1.46	1.43
3:H:132:LYS:NZ	3:H:223:THR:HG23	1.32	1.43
2:M:197:PHE:HZ	4:M:310:BCL:CBB	1.32	1.43
1:L:175:ILE:HG21	1:L:243:PHE:CE2	1.54	1.42
1:L:33:PHE:CD1	1:L:33:PHE:O	1.69	1.41
3:H:27:LEU:HD12	3:H:28:ILE:N	1.26	1.41
3:H:56:PHE:HD1	3:H:57:PRO:N	1.10	1.40
1:L:185:LEU:HD23	1:L:186:ALA:N	1.31	1.40
1:L:97:PHE:HE1	4:L:283:BCL:C14	1.35	1.39
2:M:249:ALA:HB2	6:M:313:U10:C4M	1.53	1.38
3:H:36:MET:H	3:H:36:MET:CE	1.35	1.38
2:M:218:MET:CE	2:M:252:TRP:CZ2	2.04	1.37
6:L:285:U10:C11	6:L:285:U10:H152	1.54	1.37
1:L:175:ILE:CG2	1:L:243:PHE:HD2	1.36	1.36
5:L:284:BPH:H171	5:L:284:BPH:C14	1.50	1.36
6:L:285:U10:C11	6:L:285:U10:C15	2.02	1.36
2:M:187:ASN:HD22	2:M:188:ASN:N	1.20	1.36
3:H:191:LEU:CD1	3:H:205:VAL:HG11	1.55	1.36
2:M:243:THR:HG21	2:M:247:ARG:NE	1.37	1.35
6:L:285:U10:C15	6:L:285:U10:H111	1.42	1.34
1:L:51:TRP:HD1	1:L:51:TRP:O	1.06	1.33
2:M:218:MET:HE3	2:M:252:TRP:CH2	1.60	1.33
3:H:36:MET:HE2	3:H:36:MET:N	1.37	1.33
1:L:175:ILE:CG2	1:L:243:PHE:CD2	2.07	1.33
2:M:73:TRP:NE1	2:M:114:LEU:HG	1.40	1.33
3:H:151:LEU:O	3:H:164:VAL:HG23	1.25	1.33
3:H:56:PHE:CD1	3:H:57:PRO:HD2	1.62	1.32
3:H:56:PHE:CD1	3:H:57:PRO:CD	2.12	1.32
2:M:73:TRP:CD1	2:M:114:LEU:CG	2.13	1.31
1:L:185:LEU:CD2	1:L:186:ALA:H	1.43	1.31
1:L:248:MET:HE1	4:L:283:BCL:C3D	1.61	1.30
3:H:160:ILE:CD1	3:H:160:ILE:H	1.43	1.30
2:M:35:PHE:CD2	2:M:47:LEU:CD1	2.15	1.29
2:M:64:LEU:CD1	5:M:312:BPH:H7C1	1.63	1.28
3:H:213:PHE:O	3:H:216:ILE:HD12	1.21	1.28
1:L:208:THR:CG2	1:L:211:HIS:HD2	1.46	1.27
3:H:40:TYR:O	3:H:42:LEU:HD13	1.11	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ASN:O	1:L:183:ASN:ND2	1.67	1.26
1:L:179:PHE:CB	1:L:240:ALA:HB2	1.63	1.26
1:L:234:LEU:HD23	1:L:234:LEU:O	1.20	1.26
1:L:232:LEU:HG	2:M:42:PHE:CE2	1.70	1.25
3:H:56:PHE:CD1	3:H:57:PRO:N	2.04	1.25
1:L:208:THR:CG2	1:L:211:HIS:CD2	2.20	1.24
1:L:7:ARG:O	3:H:87:LEU:HD23	1.36	1.24
2:M:51:TYR:O	2:M:51:TYR:HD1	1.22	1.23
1:L:53:ALA:HB2	1:L:64:ILE:CG1	1.68	1.23
1:L:269:LEU:CD2	1:L:270:PRO:HD3	1.69	1.23
2:M:70:ILE:HD12	7:M:308:BOG:O6	1.38	1.23
1:L:175:ILE:CD1	1:L:243:PHE:HE2	1.51	1.22
2:M:260:ALA:CA	3:H:36:MET:HG3	1.67	1.22
1:L:206:MET:N	3:H:65:ILE:HG22	1.53	1.22
1:L:185:LEU:HA	1:L:188:ALA:CB	1.70	1.21
2:M:87:ARG:HD2	2:M:88:ASP:CG	1.61	1.21
2:M:260:ALA:HA	3:H:36:MET:CG	1.70	1.21
2:M:20:MET:HG3	2:M:21:THR:N	1.39	1.20
2:M:109:LEU:HD22	2:M:110:LYS:N	1.55	1.20
1:L:73:TYR:CD2	1:L:82:LYS:HE3	1.75	1.20
3:H:20:PHE:CE1	3:H:24:LEU:HD12	1.75	1.20
2:M:187:ASN:ND2	2:M:188:ASN:N	1.85	1.20
1:L:175:ILE:CD1	1:L:243:PHE:CE2	2.24	1.20
2:M:185:TRP:CD2	2:M:185:TRP:O	1.95	1.20
3:H:40:TYR:O	3:H:42:LEU:CD1	1.88	1.20
3:H:27:LEU:HD13	3:H:32:GLN:OE1	1.41	1.19
2:M:249:ALA:CB	6:M:313:U10:C4M	2.19	1.19
3:H:27:LEU:HD22	3:H:32:GLN:HE22	1.03	1.19
2:M:87:ARG:CG	2:M:88:ASP:N	2.03	1.19
2:M:102:GLY:O	2:M:104:SER:N	1.75	1.18
3:H:111:PRO:HG2	3:H:242:MET:CB	1.73	1.18
1:L:216:PHE:CD2	6:L:285:U10:H71	1.77	1.18
1:L:51:TRP:O	1:L:51:TRP:CD1	1.96	1.17
3:H:27:LEU:CD2	3:H:32:GLN:HE22	1.55	1.17
1:L:177:ILE:HG22	1:L:181:PHE:CD2	1.79	1.17
2:M:88:ASP:HB2	2:M:92:PHE:CZ	1.79	1.17
2:M:87:ARG:HG3	2:M:88:ASP:N	1.22	1.17
3:H:27:LEU:HD13	3:H:32:GLN:CD	1.65	1.16
3:H:94:GLU:O	3:H:96:PHE:N	1.78	1.16
1:L:185:LEU:O	1:L:188:ALA:N	1.77	1.16
3:H:194:GLN:H	3:H:194:GLN:CD	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:GLY:O	1:L:151:TRP:N	1.76	1.16
2:M:46:GLN:NE2	2:M:49:PRO:HD2	1.61	1.16
3:H:179:LEU:O	3:H:179:LEU:HD23	1.44	1.16
3:H:20:PHE:CZ	3:H:24:LEU:HD12	1.80	1.16
2:M:242:GLY:HA2	3:H:115:VAL:HG11	1.28	1.15
1:L:208:THR:O	1:L:211:HIS:HB2	1.43	1.15
1:L:222:TYR:CD1	1:L:223:SER:N	2.14	1.15
1:L:269:LEU:HB3	1:L:270:PRO:HD2	1.25	1.15
2:M:204:LEU:HA	2:M:207:ALA:CB	1.77	1.15
1:L:205:GLU:HA	3:H:65:ILE:CG2	1.76	1.15
2:M:289:THR:O	2:M:291:VAL:N	1.77	1.15
6:M:313:U10:C21	6:M:313:U10:H252	1.75	1.15
6:M:313:U10:H252	6:M:313:U10:H211	1.20	1.15
1:L:269:LEU:CB	1:L:270:PRO:HD2	1.76	1.15
2:M:21:THR:HB	2:M:139:ALA:HB1	1.20	1.15
1:L:53:ALA:HB2	1:L:64:ILE:CD1	1.76	1.14
4:L:283:BCL:H143	5:L:284:BPH:HBA2	1.24	1.14
2:M:127:TRP:O	2:M:130:TRP:HB3	1.46	1.14
2:M:187:ASN:ND2	2:M:188:ASN:H	1.41	1.14
3:H:56:PHE:HD1	3:H:57:PRO:CD	1.56	1.14
1:L:133:LEU:O	1:L:137:VAL:HG23	1.47	1.14
2:M:88:ASP:C	2:M:92:PHE:CE2	2.21	1.14
3:H:124:ASP:OD1	3:H:125:GLY:N	1.78	1.14
3:H:151:LEU:O	3:H:164:VAL:CG2	1.96	1.14
1:L:224:ILE:O	1:L:225:GLY:O	1.63	1.14
2:M:131:GLY:O	2:M:134:TYR:N	1.81	1.14
2:M:196:LEU:HD13	2:M:294:TRP:CD1	1.84	1.13
2:M:204:LEU:HA	2:M:207:ALA:HB2	1.22	1.13
3:H:36:MET:CE	3:H:36:MET:N	2.01	1.13
3:H:56:PHE:HD1	3:H:56:PHE:C	1.51	1.13
1:L:206:MET:H	3:H:65:ILE:CG2	1.61	1.13
1:L:8:LYS:HA	3:H:87:LEU:CD2	1.79	1.13
1:L:21:LEU:HD12	1:L:22:PHE:CE1	1.84	1.13
4:L:283:BCL:H143	5:L:284:BPH:CBA	1.75	1.13
2:M:96:PRO:HB2	2:M:97:PRO:HD2	1.14	1.13
1:L:10:ARG:NH2	3:H:95:GLY:HA2	1.63	1.12
2:M:17:ASP:C	2:M:18:LEU:HD12	1.68	1.12
2:M:249:ALA:CB	6:M:313:U10:H4M3	1.79	1.13
6:M:313:U10:C21	6:M:313:U10:C25	2.25	1.12
3:H:27:LEU:CD1	3:H:28:ILE:N	2.11	1.12
1:L:227:LEU:HD23	1:L:231:ARG:HD2	1.21	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:261:THR:O	2:M:263:GLU:N	1.81	1.12
3:H:183:LEU:HD23	3:H:183:LEU:H	1.07	1.12
3:H:12:LEU:HD23	3:H:12:LEU:C	1.68	1.12
1:L:268:LYS:HG2	1:L:269:LEU:N	1.42	1.12
1:L:248:MET:HE1	4:L:283:BCL:C2D	1.79	1.11
2:M:101:TYR:O	2:M:101:TYR:HD1	1.33	1.11
3:H:191:LEU:HD13	3:H:205:VAL:HG11	1.16	1.11
3:H:148:PRO:O	3:H:151:LEU:HB2	1.50	1.11
1:L:234:LEU:O	1:L:234:LEU:CD2	1.98	1.10
2:M:149:ALA:O	5:M:312:BPH:HMD3	1.48	1.10
2:M:186:THR:HG23	4:M:310:BCL:HMD2	1.13	1.10
5:M:312:BPH:HBC3	5:M:312:BPH:HHD	1.32	1.10
1:L:94:THR:CG2	1:L:129:LEU:HD11	1.80	1.10
2:M:94:LEU:HD11	2:M:114:LEU:HD23	1.21	1.10
2:M:114:LEU:O	2:M:117:ILE:HB	1.48	1.10
3:H:15:LEU:HA	3:H:18:TYR:CD2	1.87	1.10
3:H:24:LEU:HD23	3:H:28:ILE:CD1	1.82	1.10
3:H:43:GLU:OE1	3:H:44:ASN:ND2	1.84	1.10
1:L:215:PHE:HE1	1:L:219:LEU:HD22	1.14	1.10
2:M:35:PHE:HD2	2:M:47:LEU:HD13	1.01	1.10
1:L:195:LEU:HB3	2:M:145:HIS:CD2	1.87	1.09
2:M:57:VAL:CG2	2:M:58:LEU:H	1.63	1.09
4:L:283:BCL:CMC	4:M:310:BCL:CBC	2.30	1.09
1:L:86:TRP:CE3	1:L:87:GLN:N	2.20	1.09
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.29	1.09
1:L:135:ARG:HG3	1:L:139:MET:HE1	1.24	1.09
2:M:243:THR:HG22	2:M:247:ARG:HG2	1.25	1.09
1:L:267:VAL:HG13	2:M:87:ARG:HD3	1.34	1.08
2:M:135:LEU:H	2:M:135:LEU:HD12	1.13	1.08
2:M:235:LEU:H	2:M:235:LEU:HD12	1.13	1.08
3:H:111:PRO:HD2	3:H:243:TYR:CE1	1.87	1.08
2:M:51:TYR:O	2:M:51:TYR:CD1	2.05	1.08
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.16	1.08
2:M:218:MET:CE	2:M:252:TRP:CH2	2.32	1.08
3:H:132:LYS:NZ	3:H:223:THR:CG2	2.17	1.08
1:L:107:ILE:HD12	2:M:255:THR:OG1	1.53	1.08
1:L:186:ALA:O	2:M:216:PHE:HE2	1.35	1.08
1:L:216:PHE:HD2	6:L:285:U10:H71	0.95	1.08
2:M:54:SER:O	2:M:57:VAL:HG13	1.51	1.07
2:M:90:PHE:HA	2:M:179:ILE:HD12	1.31	1.07
2:M:109:LEU:HD23	2:M:114:LEU:HD11	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:VAL:O	2:M:26:LEU:N	1.88	1.07
1:L:179:PHE:HB2	1:L:240:ALA:CB	1.84	1.07
1:L:215:PHE:CE1	1:L:219:LEU:HD22	1.87	1.07
1:L:231:ARG:NH2	2:M:7:PHE:HA	1.67	1.07
1:L:93:ALA:O	1:L:95:GLY:N	1.86	1.07
1:L:205:GLU:HA	3:H:65:ILE:HG21	1.29	1.07
2:M:37:THR:HG22	2:M:38:LEU:HD12	1.34	1.07
3:H:24:LEU:HD23	3:H:28:ILE:HD11	1.14	1.07
1:L:20:ASN:O	1:L:22:PHE:N	1.87	1.06
1:L:182:THR:O	1:L:185:LEU:CD2	2.03	1.06
2:M:299:GLN:HE21	2:M:299:GLN:HA	1.13	1.06
3:H:14:SER:O	3:H:18:TYR:HB3	1.51	1.06
1:L:232:LEU:HG	2:M:42:PHE:CZ	1.90	1.06
1:L:242:PHE:HD1	1:L:243:PHE:N	1.51	1.06
3:H:37:ARG:NH2	3:H:41:PRO:O	1.87	1.06
1:L:178:SER:HB2	4:L:282:BCL:O1A	1.50	1.06
2:M:206:ILE:HD11	4:M:310:BCL:C1B	1.85	1.06
2:M:46:GLN:HG2	2:M:47:LEU:H	1.21	1.06
3:H:191:LEU:CD1	3:H:205:VAL:CG1	2.32	1.06
3:H:210:SER:O	3:H:212:LEU:N	1.88	1.06
1:L:219:LEU:HD21	2:M:133:THR:HG23	1.34	1.06
2:M:218:MET:HE2	2:M:252:TRP:CE2	1.90	1.05
1:L:21:LEU:HD12	1:L:22:PHE:HE1	1.13	1.05
3:H:160:ILE:HD12	3:H:160:ILE:N	1.69	1.05
3:H:161:ALA:HB2	3:H:210:SER:HB2	1.31	1.05
3:H:191:LEU:HD13	3:H:205:VAL:CG1	1.84	1.05
3:H:157:ASP:OD2	3:H:211:ASP:HB2	1.56	1.05
1:L:5:PHE:HZ	3:H:40:TYR:CE2	1.73	1.05
2:M:218:MET:CE	2:M:252:TRP:CE2	2.39	1.05
3:H:27:LEU:HD22	3:H:32:GLN:NE2	1.70	1.05
2:M:64:LEU:HD11	5:M:312:BPH:H7C1	1.38	1.05
3:H:189:ARG:HB2	3:H:216:ILE:HG21	1.30	1.05
4:L:283:BCL:CMC	4:M:310:BCL:HBC1	1.87	1.04
2:M:185:TRP:O	2:M:185:TRP:CE3	2.09	1.04
4:L:283:BCL:H151	5:L:284:BPH:H3A	1.35	1.04
1:L:49:ILE:HG22	1:L:50:ALA:H	1.20	1.04
3:H:215:GLY:HA3	3:H:236:TYR:CZ	1.92	1.04
1:L:94:THR:OG1	1:L:129:LEU:CD1	2.03	1.04
6:L:285:U10:C8	6:L:285:U10:H1M1	1.87	1.04
4:L:283:BCL:HBD	4:M:311:BCL:HBC1	1.36	1.04
2:M:35:PHE:CD2	2:M:47:LEU:HD11	1.91	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:135:LEU:HB3	2:M:138:GLN:OE1	1.57	1.04
1:L:8:LYS:CA	3:H:87:LEU:HD22	1.88	1.03
1:L:79:PRO:O	1:L:81:ALA:N	1.89	1.03
1:L:177:ILE:CG2	1:L:181:PHE:CE2	2.41	1.03
1:L:183:ASN:ND2	1:L:183:ASN:C	2.10	1.03
1:L:185:LEU:HA	1:L:188:ALA:HB2	1.38	1.03
1:L:187:LEU:HD22	2:M:216:PHE:CG	1.92	1.03
1:L:269:LEU:CD2	1:L:270:PRO:CD	2.28	1.03
3:H:210:SER:OG	3:H:211:ASP:OD1	1.76	1.03
1:L:193:LEU:HD23	6:L:285:U10:C3	1.89	1.03
2:M:39:LEU:HD13	2:M:39:LEU:N	1.71	1.03
3:H:151:LEU:HD22	3:H:203:VAL:CG2	1.89	1.03
3:H:170:ASP:OD2	3:H:177:ARG:NH2	1.92	1.03
1:L:73:TYR:HB2	1:L:82:LYS:NZ	1.72	1.02
2:M:228:ARG:HH11	2:M:228:ARG:HG2	0.88	1.02
1:L:73:TYR:HB2	1:L:82:LYS:HZ1	1.20	1.02
1:L:86:TRP:HE3	1:L:87:GLN:N	1.55	1.02
1:L:241:VAL:O	1:L:244:SER:HB2	1.57	1.02
2:M:35:PHE:CD2	2:M:47:LEU:HD13	1.84	1.02
2:M:114:LEU:CD1	2:M:114:LEU:H	1.73	1.02
2:M:238:ILE:HG23	2:M:238:ILE:O	1.55	1.02
1:L:73:TYR:CD2	1:L:82:LYS:CE	2.41	1.02
1:L:242:PHE:CD1	1:L:243:PHE:N	2.26	1.02
2:M:65:MET:HG2	2:M:66:TRP:N	1.74	1.02
2:M:243:THR:CG2	2:M:247:ARG:NE	2.06	1.02
3:H:17:ILE:CD1	3:H:17:ILE:O	2.07	1.02
1:L:135:ARG:HH12	1:L:252:GLY:HA3	0.90	1.02
2:M:299:GLN:HA	2:M:299:GLN:NE2	1.64	1.02
6:M:313:U10:C25	6:M:313:U10:H212	1.89	1.02
3:H:151:LEU:HD22	3:H:203:VAL:HG23	1.41	1.02
3:H:238:ALA:O	3:H:240:GLY:N	1.93	1.02
1:L:53:ALA:HB2	1:L:64:ILE:HG12	1.40	1.02
1:L:60:ASN:O	1:L:62:GLN:N	1.92	1.02
3:H:116:ALA:HA	3:H:228:LEU:CD1	1.90	1.02
3:H:195:MET:C	3:H:196:VAL:HG13	1.78	1.02
1:L:135:ARG:NH1	1:L:252:GLY:HA3	1.75	1.01
2:M:64:LEU:HD12	5:M:312:BPH:H7C1	1.37	1.01
2:M:228:ARG:HG2	2:M:228:ARG:NH1	1.72	1.01
3:H:160:ILE:CD1	3:H:160:ILE:N	2.16	1.01
1:L:71:LEU:O	1:L:73:TYR:N	1.94	1.01
2:M:214:LEU:O	2:M:217:ALA:HB3	1.57	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:OG	1:L:67:TYR:HE1	1.44	1.01
1:L:267:VAL:CG1	2:M:87:ARG:HD3	1.89	1.01
4:L:283:BCL:HMC1	4:M:310:BCL:HBC1	1.42	1.01
2:M:196:LEU:CD1	2:M:294:TRP:CD1	2.42	1.01
2:M:204:LEU:CA	2:M:207:ALA:HB2	1.90	1.01
2:M:205:SER:OG	2:M:279:THR:HG22	1.61	1.01
2:M:257:GLY:O	2:M:258:PHE:HB3	1.56	1.01
1:L:8:LYS:HA	3:H:87:LEU:HD22	1.01	1.01
1:L:179:PHE:HB2	1:L:240:ALA:HB2	1.01	1.01
2:M:54:SER:O	2:M:57:VAL:CG1	2.08	1.01
2:M:218:MET:HE3	2:M:252:TRP:CZ3	1.96	1.01
3:H:156:CYS:SG	3:H:209:SER:HA	2.01	1.01
1:L:5:PHE:CZ	3:H:40:TYR:CE2	2.49	1.00
2:M:228:ARG:HH11	2:M:228:ARG:CG	1.70	1.00
3:H:134:MET:HE2	3:H:167:ILE:HB	1.39	1.00
2:M:87:ARG:HD2	2:M:88:ASP:OD1	1.59	1.00
3:H:36:MET:H	3:H:36:MET:HE3	1.24	1.00
1:L:151:TRP:HH2	2:M:198:TYR:HA	1.24	1.00
2:M:249:ALA:CB	6:M:313:U10:H4M1	1.85	1.00
3:H:160:ILE:H	3:H:160:ILE:HD13	1.23	1.00
1:L:11:VAL:HG21	3:H:110:GLY:HA2	1.04	1.00
1:L:49:ILE:CG2	1:L:50:ALA:H	1.74	1.00
2:M:96:PRO:CB	2:M:97:PRO:HD2	1.91	1.00
2:M:99:PRO:HB2	2:M:111:GLU:CG	1.92	1.00
2:M:46:GLN:NE2	2:M:49:PRO:CD	2.24	1.00
1:L:17:VAL:HG13	1:L:18:GLY:H	1.27	1.00
1:L:224:ILE:HD12	1:L:232:LEU:HD12	1.42	0.99
2:M:16:ALA:HB1	2:M:32:VAL:HG21	1.43	0.99
2:M:299:GLN:HE21	2:M:299:GLN:CA	1.69	0.99
1:L:65:SER:OG	1:L:67:TYR:CE1	2.15	0.99
2:M:208:PHE:O	2:M:211:GLY:N	1.94	0.99
2:M:110:LYS:HE2	2:M:114:LEU:HD21	1.44	0.99
2:M:20:MET:CG	2:M:21:THR:N	2.25	0.99
2:M:46:GLN:HE22	2:M:49:PRO:HD2	1.26	0.99
1:L:51:TRP:HD1	1:L:51:TRP:C	1.65	0.99
1:L:97:PHE:CZ	4:L:283:BCL:H122	1.98	0.99
1:L:153:HIS:HD2	1:L:154:LEU:HD12	1.24	0.99
2:M:243:THR:HG21	2:M:247:ARG:CZ	1.91	0.99
1:L:237:SER:O	1:L:239:SER:N	1.96	0.98
2:M:37:THR:HG22	2:M:38:LEU:CD1	1.90	0.98
1:L:11:VAL:HG12	3:H:87:LEU:HD11	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ALA:HB2	1:L:64:ILE:HD13	1.43	0.98
1:L:204:LYS:HB3	1:L:207:ARG:HH12	1.25	0.98
2:M:100:GLU:HA	2:M:172:SER:OG	1.63	0.98
2:M:119:SER:HA	2:M:177:TYR:OH	1.63	0.98
2:M:35:PHE:CD1	2:M:38:LEU:HB2	1.98	0.98
2:M:57:VAL:HG22	2:M:58:LEU:H	1.27	0.98
3:H:183:LEU:HD11	3:H:189:ARG:HE	1.23	0.98
1:L:11:VAL:HG21	3:H:110:GLY:CA	1.92	0.98
2:M:186:THR:CG2	4:M:310:BCL:HMD2	1.93	0.98
1:L:22:PHE:HE2	1:L:36:VAL:HG11	1.26	0.97
1:L:227:LEU:CD2	1:L:231:ARG:HD2	1.94	0.97
2:M:226:VAL:HG12	2:M:231:GLY:HA3	1.44	0.97
3:H:42:LEU:HD23	3:H:77:GLY:H	1.25	0.97
3:H:189:ARG:HB3	3:H:189:ARG:HH11	1.24	0.97
1:L:102:LEU:HD23	1:L:102:LEU:H	1.29	0.97
1:L:219:LEU:HA	2:M:132:ARG:HH21	1.26	0.97
2:M:94:LEU:HD21	2:M:114:LEU:HB3	1.45	0.97
3:H:116:ALA:HA	3:H:228:LEU:HG	1.46	0.97
1:L:154:LEU:HD23	2:M:197:PHE:HB3	1.42	0.97
1:L:231:ARG:CZ	2:M:7:PHE:HA	1.94	0.97
1:L:34:PHE:O	1:L:38:THR:N	1.97	0.97
1:L:135:ARG:CG	1:L:139:MET:HE1	1.94	0.97
1:L:183:ASN:HB2	1:L:236:LEU:HB2	1.44	0.97
1:L:208:THR:CB	1:L:211:HIS:HD2	1.76	0.97
2:M:238:ILE:O	2:M:238:ILE:CG2	2.13	0.97
1:L:180:PHE:HE1	2:M:213:ALA:HB2	1.29	0.96
2:M:27:ALA:O	2:M:28:ASN:OD1	1.83	0.96
2:M:46:GLN:CG	2:M:47:LEU:H	1.69	0.96
2:M:152:SER:C	2:M:277:THR:HG21	1.85	0.96
2:M:164:ARG:NH2	2:M:168:MET:HE1	1.80	0.96
2:M:241:ARG:HB3	2:M:241:ARG:HH11	1.29	0.96
1:L:268:LYS:HG2	1:L:269:LEU:H	0.88	0.96
2:M:203:GLY:O	2:M:207:ALA:N	1.97	0.96
2:M:237:GLN:OE1	2:M:244:ALA:HB3	1.65	0.96
1:L:177:ILE:HG22	1:L:181:PHE:CE2	2.00	0.96
2:M:21:THR:OG1	2:M:23:ASP:O	1.83	0.96
3:H:210:SER:OG	3:H:211:ASP:N	1.93	0.96
1:L:156:TRP:CE3	1:L:156:TRP:C	2.39	0.96
2:M:108:PRO:HG2	2:M:111:GLU:HB3	1.48	0.96
2:M:209:LEU:O	2:M:209:LEU:HD13	1.65	0.96
4:L:283:BCL:C4	5:L:284:BPH:CAB	2.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215:PHE:O	1:L:218:ASP:HB2	1.63	0.96
2:M:204:LEU:O	2:M:207:ALA:N	1.98	0.96
1:L:49:ILE:CG2	1:L:50:ALA:N	2.26	0.95
1:L:135:ARG:HH12	1:L:252:GLY:CA	1.79	0.95
2:M:59:SER:OG	2:M:129:TRP:HB2	1.66	0.95
1:L:128:TYR:O	1:L:130:THR:N	1.99	0.95
1:L:185:LEU:HA	1:L:188:ALA:HB3	1.46	0.95
2:M:96:PRO:HB2	2:M:97:PRO:CD	1.96	0.95
3:H:111:PRO:HG3	3:H:242:MET:HG3	1.44	0.95
2:M:109:LEU:HD22	2:M:109:LEU:C	1.85	0.95
3:H:151:LEU:HB3	3:H:203:VAL:HG21	1.45	0.95
1:L:48:LEU:HD11	1:L:89:ILE:HG13	1.48	0.95
2:M:253:ARG:HG2	2:M:259:ASN:OD1	1.67	0.95
3:H:189:ARG:HD3	3:H:216:ILE:HB	1.48	0.95
2:M:15:PRO:HD2	3:H:140:PHE:CE1	2.00	0.95
2:M:122:MET:O	2:M:122:MET:HG2	1.65	0.95
2:M:268:TRP:CD1	6:M:313:U10:H111	2.02	0.95
2:M:197:PHE:CZ	4:M:310:BCL:CBB	2.19	0.94
2:M:73:TRP:NE1	2:M:114:LEU:CG	2.23	0.94
2:M:249:ALA:HB2	6:M:313:U10:H4M1	0.98	0.94
3:H:17:ILE:O	3:H:17:ILE:HD12	1.65	0.94
3:H:183:LEU:H	3:H:183:LEU:CD2	1.79	0.94
1:L:24:PHE:CE2	1:L:31:VAL:HG21	2.02	0.94
1:L:232:LEU:HG	2:M:42:PHE:HE2	1.31	0.94
6:L:285:U10:H303	6:L:285:U10:H261	1.48	0.94
1:L:186:ALA:O	2:M:216:PHE:CE2	2.20	0.94
3:H:195:MET:O	3:H:196:VAL:HG22	1.67	0.94
1:L:232:LEU:HA	2:M:42:PHE:HZ	1.32	0.94
1:L:241:VAL:HG12	1:L:242:PHE:N	1.81	0.94
2:M:164:ARG:NH2	2:M:168:MET:CE	2.30	0.94
1:L:135:ARG:HH11	1:L:139:MET:HE1	1.31	0.94
2:M:209:LEU:N	2:M:276:VAL:HG22	1.82	0.94
3:H:160:ILE:H	3:H:160:ILE:HD12	1.26	0.94
3:H:24:LEU:CD2	3:H:28:ILE:HD11	1.96	0.94
2:M:135:LEU:HD12	2:M:135:LEU:N	1.81	0.93
1:L:133:LEU:HD12	1:L:133:LEU:C	1.88	0.93
2:M:101:TYR:O	2:M:101:TYR:CD1	2.20	0.93
2:M:67:PHE:CD1	2:M:67:PHE:C	2.39	0.93
3:H:19:SER:O	3:H:22:ILE:N	2.02	0.93
1:L:97:PHE:CE1	4:L:283:BCL:C14	2.25	0.93
1:L:156:TRP:CE3	1:L:156:TRP:O	2.20	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:HIS:O	1:L:169:TYR:HD1	1.52	0.93
2:M:16:ALA:CB	2:M:32:VAL:HG21	1.99	0.93
2:M:227:SER:HB3	3:H:194:GLN:HG2	1.50	0.93
4:L:283:BCL:CMC	4:M:310:BCL:HBC2	1.98	0.93
2:M:46:GLN:NE2	2:M:48:GLY:O	2.02	0.93
3:H:133:PRO:HD2	3:H:136:ALA:HB3	1.49	0.93
1:L:97:PHE:HE1	4:L:283:BCL:H142	0.83	0.93
1:L:268:LYS:CG	1:L:269:LEU:H	1.81	0.93
2:M:138:GLN:O	2:M:141:GLY:N	2.00	0.93
2:M:164:ARG:O	2:M:167:LEU:N	2.02	0.93
1:L:60:ASN:HB3	1:L:63:LEU:HD12	1.51	0.93
1:L:6:GLU:OE2	1:L:10:ARG:HD3	1.69	0.93
2:M:290:VAL:O	2:M:291:VAL:HG23	1.69	0.93
3:H:247:LYS:C	3:H:248:ARG:HG3	1.89	0.93
1:L:93:ALA:HB1	1:L:97:PHE:CE2	2.03	0.92
1:L:237:SER:OG	1:L:238:LEU:N	1.99	0.92
1:L:154:LEU:HD12	1:L:154:LEU:H	1.30	0.92
2:M:73:TRP:CG	2:M:114:LEU:HG	2.03	0.92
2:M:264:GLY:HA2	2:M:267:ARG:HB2	1.51	0.92
3:H:179:LEU:O	3:H:179:LEU:CD2	2.17	0.92
3:H:210:SER:C	3:H:212:LEU:H	1.71	0.92
1:L:12:PRO:HD2	3:H:98:HIS:O	1.70	0.92
1:L:153:HIS:CD2	1:L:154:LEU:HD12	2.05	0.92
2:M:170:SER:OG	2:M:172:SER:CB	2.17	0.92
3:H:154:ARG:NE	3:H:160:ILE:HG13	1.84	0.92
1:L:175:ILE:HG22	1:L:243:PHE:HD2	1.33	0.92
2:M:26:LEU:HD23	2:M:27:ALA:H	1.34	0.92
2:M:67:PHE:C	2:M:67:PHE:HD1	1.70	0.92
2:M:170:SER:OG	2:M:172:SER:HB2	1.69	0.92
2:M:164:ARG:CB	2:M:165:PRO:HD3	1.99	0.92
3:H:190:LEU:HD23	3:H:190:LEU:H	1.30	0.92
1:L:146:PHE:HB2	1:L:147:PRO:HD2	1.49	0.92
2:M:17:ASP:CA	2:M:18:LEU:HD12	2.00	0.92
2:M:164:ARG:HB3	2:M:165:PRO:CD	2.00	0.92
3:H:148:PRO:O	3:H:164:VAL:HG21	1.67	0.92
1:L:43:ALA:O	1:L:45:GLY:N	2.01	0.92
2:M:90:PHE:CD2	2:M:180:PHE:CE1	2.57	0.92
3:H:194:GLN:CD	3:H:194:GLN:N	2.19	0.92
1:L:214:THR:HG22	2:M:140:LEU:HD21	1.52	0.91
3:H:183:LEU:CD1	3:H:189:ARG:HE	1.82	0.91
3:H:213:PHE:O	3:H:216:ILE:CD1	2.14	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:228:LEU:CD2	3:H:232:LYS:HD2	2.00	0.91
1:L:151:TRP:CH2	2:M:198:TYR:HA	2.05	0.91
1:L:39:PHE:O	1:L:41:PHE:N	2.02	0.91
1:L:86:TRP:HE3	1:L:87:GLN:H	1.08	0.91
1:L:113:ILE:HD11	2:M:226:VAL:HG22	1.49	0.91
3:H:61:PRO:HA	3:H:76:PRO:HG2	1.52	0.91
3:H:124:ASP:OD1	3:H:124:ASP:C	2.09	0.91
3:H:183:LEU:HD23	3:H:183:LEU:N	1.84	0.91
3:H:20:PHE:O	3:H:22:ILE:N	2.03	0.91
3:H:111:PRO:HG2	3:H:242:MET:HB3	1.51	0.91
3:H:161:ALA:HB2	3:H:210:SER:CB	1.99	0.91
1:L:133:LEU:CD1	1:L:137:VAL:HG21	2.00	0.91
2:M:87:ARG:CD	2:M:88:ASP:CG	2.38	0.91
3:H:94:GLU:C	3:H:96:PHE:H	1.68	0.91
1:L:6:GLU:O	1:L:9:TYR:N	2.04	0.91
1:L:167:PHE:HD2	4:L:283:BCL:CHD	1.82	0.91
2:M:204:LEU:CA	2:M:207:ALA:CB	2.47	0.91
3:H:211:ASP:O	3:H:212:LEU:HD12	1.71	0.91
1:L:97:PHE:CE1	4:L:283:BCL:H111	2.06	0.91
2:M:159:VAL:O	2:M:161:GLY:N	2.02	0.91
3:H:27:LEU:CD1	3:H:32:GLN:OE1	2.19	0.91
1:L:49:ILE:O	1:L:52:SER:N	2.03	0.91
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.06	0.91
2:M:94:LEU:CD1	2:M:114:LEU:HD23	2.00	0.91
3:H:27:LEU:CD1	3:H:28:ILE:H	1.73	0.91
2:M:284:ILE:HD12	4:M:310:BCL:O2D	1.72	0.90
1:L:135:ARG:HG3	1:L:139:MET:CE	2.02	0.90
1:L:269:LEU:CG	1:L:270:PRO:HD2	2.00	0.90
3:H:110:GLY:O	3:H:113:SER:OG	1.86	0.90
3:H:155:GLY:O	3:H:204:HIS:HD2	1.55	0.90
1:L:94:THR:OG1	1:L:129:LEU:HD11	1.72	0.90
1:L:171:PRO:O	1:L:173:HIS:N	2.04	0.90
1:L:156:TRP:HE3	1:L:157:VAL:N	1.70	0.90
4:L:283:BCL:HMC2	4:M:310:BCL:CBC	2.02	0.90
2:M:243:THR:HG22	2:M:247:ARG:CG	2.01	0.90
2:M:249:ALA:HA	6:M:313:U10:H4M3	1.53	0.90
1:L:33:PHE:O	1:L:33:PHE:HD1	1.44	0.90
2:M:87:ARG:CG	2:M:88:ASP:H	1.84	0.90
1:L:187:LEU:HD22	2:M:216:PHE:CD2	2.07	0.90
1:L:232:LEU:O	1:L:235:LEU:HB2	1.70	0.90
4:M:311:BCL:CBB	4:M:311:BCL:HMB1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:173:GLU:HB3	3:H:175:MET:HG3	1.52	0.90
3:H:20:PHE:CE1	3:H:24:LEU:CD1	2.55	0.90
2:M:105:PHE:CD1	2:M:106:ALA:N	2.39	0.90
1:L:147:PRO:HG2	1:L:152:THR:HG22	1.52	0.90
1:L:152:THR:O	1:L:155:ASP:N	2.05	0.90
1:L:156:TRP:CE3	1:L:157:VAL:HA	2.07	0.90
2:M:35:PHE:CG	2:M:39:LEU:CD2	2.55	0.90
2:M:57:VAL:CG2	2:M:58:LEU:N	2.27	0.90
2:M:243:THR:HG22	2:M:247:ARG:HE	1.34	0.90
3:H:39:GLY:HA2	3:H:42:LEU:HD21	1.51	0.90
3:H:116:ALA:HA	3:H:228:LEU:CG	2.02	0.90
2:M:13:ARG:HA	3:H:174:GLN:HG2	1.52	0.89
2:M:99:PRO:HB2	2:M:111:GLU:CD	1.93	0.89
1:L:10:ARG:HH22	3:H:95:GLY:HA2	1.34	0.89
1:L:248:MET:O	1:L:251:THR:N	2.04	0.89
6:L:285:U10:C15	6:L:285:U10:H112	2.02	0.89
3:H:97:PRO:O	3:H:98:HIS:CD2	2.26	0.89
1:L:64:ILE:HD12	1:L:65:SER:N	1.87	0.89
2:M:114:LEU:H	2:M:114:LEU:HD12	1.37	0.89
2:M:208:PHE:HB3	2:M:276:VAL:HG23	1.52	0.89
3:H:27:LEU:CD1	3:H:28:ILE:HG13	2.02	0.89
2:M:105:PHE:HD1	2:M:106:ALA:N	1.69	0.89
3:H:63:THR:HG23	3:H:74:THR:HG23	1.55	0.89
2:M:60:LEU:HD12	5:M:312:BPH:H6C1	1.54	0.89
3:H:161:ALA:CB	3:H:210:SER:HB2	2.02	0.89
3:H:191:LEU:HD11	3:H:205:VAL:HG11	1.54	0.89
7:M:308:BOG:O2	7:M:308:BOG:H5	1.71	0.89
3:H:204:HIS:ND1	3:H:205:VAL:N	2.20	0.89
1:L:255:TRP:CD1	1:L:259:TRP:CE3	2.61	0.89
2:M:39:LEU:HD13	2:M:39:LEU:H	1.32	0.89
2:M:57:VAL:HG23	2:M:58:LEU:N	1.85	0.89
3:H:179:LEU:HD23	3:H:179:LEU:C	1.92	0.89
3:H:151:LEU:HB3	3:H:203:VAL:CG2	2.01	0.89
1:L:17:VAL:HG13	1:L:18:GLY:N	1.85	0.89
2:M:90:PHE:CE2	2:M:180:PHE:CE1	2.61	0.89
1:L:9:TYR:OH	2:M:246:GLU:OE1	1.90	0.88
2:M:24:VAL:HG12	2:M:26:LEU:HD22	1.54	0.88
1:L:234:LEU:HD12	2:M:221:ALA:HA	1.54	0.88
1:L:248:MET:O	1:L:250:ILE:N	2.07	0.88
2:M:88:ASP:CB	2:M:92:PHE:CZ	2.56	0.88
2:M:233:ARG:NH2	3:H:122:GLU:OE1	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:285:U10:C11	6:L:285:U10:H153	2.02	0.88
1:L:51:TRP:CD1	1:L:51:TRP:C	2.33	0.88
3:H:56:PHE:CD1	3:H:56:PHE:C	2.25	0.88
1:L:177:ILE:HG22	1:L:181:PHE:HD2	1.37	0.88
2:M:65:MET:SD	2:M:121:PHE:HB3	2.11	0.88
3:H:114:TRP:HD1	3:H:115:VAL:O	1.57	0.88
1:L:17:VAL:CG1	1:L:18:GLY:H	1.87	0.88
1:L:94:THR:HG23	1:L:129:LEU:HD11	1.56	0.88
2:M:275:LEU:HD12	2:M:278:LEU:HD23	1.54	0.88
1:L:103:ARG:HG2	1:L:103:ARG:HH11	1.39	0.88
2:M:87:ARG:HG3	2:M:88:ASP:H	1.39	0.88
2:M:249:ALA:CA	6:M:313:U10:H4M3	2.04	0.88
3:H:40:TYR:H	3:H:42:LEU:CD1	1.86	0.88
3:H:140:PHE:CD2	3:H:169:VAL:HG11	2.09	0.88
3:H:183:LEU:HD11	3:H:189:ARG:NE	1.88	0.88
1:L:20:ASN:C	1:L:22:PHE:H	1.74	0.88
1:L:171:PRO:HA	1:L:174:MET:HG3	1.54	0.88
3:H:132:LYS:HZ1	3:H:223:THR:HG23	1.34	0.88
3:H:191:LEU:HD23	3:H:213:PHE:HE1	1.39	0.88
2:M:171:TRP:C	2:M:173:GLU:H	1.74	0.88
2:M:241:ARG:HH11	2:M:241:ARG:CB	1.86	0.88
2:M:87:ARG:HG3	2:M:88:ASP:CA	2.04	0.87
2:M:88:ASP:HB2	2:M:92:PHE:CE1	2.09	0.87
2:M:149:ALA:O	5:M:312:BPH:HMD1	1.74	0.87
3:H:134:MET:SD	3:H:141:HIS:CE1	2.68	0.87
1:L:170:ASN:O	1:L:173:HIS:HB3	1.73	0.87
1:L:269:LEU:CB	1:L:270:PRO:CD	2.53	0.87
2:M:33:GLY:O	2:M:34:PRO:O	1.91	0.87
3:H:132:LYS:HZ1	3:H:223:THR:CG2	1.83	0.87
1:L:227:LEU:HD23	1:L:231:ARG:CD	2.03	0.87
2:M:65:MET:CE	2:M:121:PHE:HB3	2.05	0.87
2:M:163:ILE:O	2:M:166:ILE:HB	1.72	0.87
2:M:291:VAL:O	2:M:291:VAL:HG12	1.74	0.87
1:L:133:LEU:CD1	1:L:137:VAL:CG2	2.53	0.87
2:M:152:SER:O	2:M:154:ILE:N	2.08	0.87
3:H:15:LEU:HA	3:H:18:TYR:CE2	2.08	0.87
1:L:232:LEU:CG	2:M:42:PHE:CE2	2.58	0.87
1:L:268:LYS:CG	1:L:269:LEU:N	2.30	0.87
3:H:97:PRO:O	3:H:98:HIS:HD2	1.58	0.87
2:M:94:LEU:HD11	2:M:114:LEU:CD2	2.02	0.87
2:M:155:TRP:O	2:M:159:VAL:HG23	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:CYS:SG	3:H:209:SER:CA	2.62	0.87
2:M:81:ASN:OD1	2:M:84:VAL:HG23	1.75	0.87
1:L:73:TYR:HD2	1:L:82:LYS:HE3	1.36	0.86
1:L:73:TYR:CB	1:L:82:LYS:HZ1	1.87	0.86
1:L:185:LEU:C	1:L:188:ALA:H	1.76	0.86
2:M:197:PHE:HE1	4:M:311:BCL:CMD	1.87	0.86
3:H:12:LEU:C	3:H:12:LEU:CD2	2.41	0.86
2:M:63:GLY:HA3	5:M:312:BPH:H5C1	1.57	0.86
1:L:60:ASN:O	1:L:61:PRO:C	2.13	0.86
3:H:111:PRO:CG	3:H:242:MET:HG3	2.04	0.86
1:L:222:TYR:CG	1:L:223:SER:N	2.32	0.86
2:M:99:PRO:HB2	2:M:111:GLU:HG3	1.57	0.86
2:M:296:VAL:O	2:M:298:GLY:N	2.09	0.86
3:H:191:LEU:CD2	3:H:213:PHE:CE1	2.59	0.86
2:M:204:LEU:O	2:M:207:ALA:HB3	1.75	0.86
2:M:65:MET:O	2:M:69:THR:N	2.08	0.86
2:M:148:TRP:O	2:M:150:PHE:N	2.09	0.86
2:M:241:ARG:HH12	2:M:246:GLU:HG2	1.40	0.86
1:L:53:ALA:CB	1:L:64:ILE:CG1	2.53	0.86
1:L:185:LEU:C	1:L:187:LEU:H	1.79	0.86
3:H:40:TYR:O	3:H:42:LEU:N	2.07	0.86
3:H:132:LYS:HD2	3:H:133:PRO:HD3	1.57	0.86
1:L:151:TRP:CZ3	1:L:154:LEU:HD22	2.11	0.86
1:L:73:TYR:CD2	1:L:82:LYS:NZ	2.44	0.85
4:L:283:BCL:H2C	4:M:310:BCL:HBC2	1.58	0.85
2:M:89:LEU:N	2:M:92:PHE:CE2	2.43	0.85
2:M:136:ARG:HA	2:M:136:ARG:HE	1.41	0.85
4:L:283:BCL:HMC1	4:M:310:BCL:CBC	2.01	0.85
2:M:126:VAL:CG1	2:M:154:ILE:HD11	2.05	0.85
2:M:271:TRP:CZ3	3:H:31:LEU:HD23	2.10	0.85
1:L:177:ILE:CG2	1:L:181:PHE:CD2	2.57	0.85
2:M:81:ASN:CG	2:M:84:VAL:HG23	1.96	0.85
2:M:199:ASN:ND2	2:M:294:TRP:CE2	2.44	0.85
3:H:111:PRO:CG	3:H:242:MET:CB	2.55	0.85
3:H:191:LEU:HD11	3:H:205:VAL:CG1	2.05	0.85
2:M:185:TRP:CE3	2:M:185:TRP:C	2.50	0.85
2:M:187:ASN:O	2:M:190:SER:N	2.10	0.85
1:L:53:ALA:CB	1:L:64:ILE:HD13	2.06	0.85
3:H:115:VAL:CG1	3:H:116:ALA:H	1.90	0.85
3:H:189:ARG:HB2	3:H:216:ILE:CG2	2.05	0.85
3:H:229:GLU:O	3:H:233:ILE:HG12	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:17:ASP:C	2:M:18:LEU:CD1	2.45	0.85
2:M:37:THR:HA	2:M:41:TRP:CD1	2.12	0.85
2:M:131:GLY:O	2:M:134:TYR:CB	2.23	0.85
2:M:280:GLY:O	4:M:310:BCL:HED3	1.76	0.85
2:M:226:VAL:CG1	2:M:231:GLY:HA3	2.05	0.85
3:H:42:LEU:CD2	3:H:76:PRO:HA	2.05	0.85
3:H:132:LYS:HZ2	3:H:223:THR:HG23	0.96	0.85
1:L:121:PHE:O	1:L:124:ALA:N	2.10	0.85
2:M:103:LEU:HD11	2:M:166:ILE:HG12	1.58	0.85
2:M:226:VAL:HG21	2:M:248:ALA:HB2	1.58	0.85
3:H:219:ILE:CG2	3:H:229:GLU:HG2	2.07	0.85
3:H:175:MET:SD	3:H:177:ARG:NH1	2.50	0.85
2:M:70:ILE:CD1	7:M:308:BOG:O6	2.25	0.85
4:M:311:BCL:O1A	4:M:311:BCL:H43	1.76	0.85
6:M:313:U10:H212	6:M:313:U10:H253	1.55	0.85
1:L:248:MET:C	1:L:250:ILE:N	2.30	0.84
2:M:99:PRO:CB	2:M:111:GLU:HG3	2.07	0.84
6:L:285:U10:H1M1	6:L:285:U10:H8	1.57	0.84
3:H:157:ASP:OD2	3:H:211:ASP:CB	2.25	0.84
2:M:94:LEU:HD21	2:M:114:LEU:CB	2.06	0.84
1:L:185:LEU:CA	1:L:188:ALA:HB3	2.07	0.84
3:H:42:LEU:HD23	3:H:77:GLY:N	1.91	0.84
1:L:10:ARG:NH2	1:L:25:TRP:HB2	1.90	0.84
1:L:133:LEU:O	1:L:133:LEU:HD12	1.78	0.84
2:M:50:ILE:HG23	2:M:51:TYR:N	1.92	0.84
2:M:212:SER:O	2:M:214:LEU:N	2.10	0.84
3:H:103:ASP:OD1	3:H:106:LYS:NZ	2.09	0.84
3:H:228:LEU:HD23	3:H:232:LYS:HD2	1.58	0.84
1:L:10:ARG:NH2	3:H:95:GLY:CA	2.41	0.84
2:M:235:LEU:HD12	2:M:235:LEU:N	1.91	0.84
3:H:183:LEU:CD2	3:H:183:LEU:N	2.37	0.84
6:L:285:U10:H8	6:L:285:U10:C1M	2.07	0.84
2:M:243:THR:HG21	2:M:247:ARG:HE	0.68	0.84
1:L:48:LEU:CD1	1:L:89:ILE:HG13	2.07	0.84
3:H:196:VAL:HA	3:H:204:HIS:O	1.77	0.84
1:L:68:PRO:HB3	1:L:86:TRP:CE2	2.13	0.84
1:L:191:GLY:O	1:L:195:LEU:HD12	1.78	0.84
1:L:11:VAL:CG2	3:H:110:GLY:HA2	2.00	0.84
1:L:248:MET:CE	4:L:283:BCL:C3D	2.53	0.84
2:M:21:THR:HB	2:M:139:ALA:CB	2.06	0.84
2:M:64:LEU:HD11	5:M:312:BPH:C7	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:MET:O	3:H:137:ALA:HB3	1.78	0.83
1:L:154:LEU:H	1:L:154:LEU:CD1	1.92	0.83
1:L:146:PHE:CB	1:L:156:TRP:CD1	2.61	0.83
2:M:275:LEU:O	2:M:277:THR:N	2.10	0.83
3:H:233:ILE:O	3:H:237:VAL:HG22	1.78	0.83
2:M:85:PHE:CE1	2:M:89:LEU:HD12	2.12	0.83
3:H:191:LEU:CD2	3:H:213:PHE:HE1	1.92	0.83
1:L:53:ALA:HB1	1:L:64:ILE:HB	1.58	0.83
2:M:89:LEU:HA	2:M:92:PHE:CD2	2.12	0.83
3:H:213:PHE:C	3:H:216:ILE:HD12	1.98	0.83
1:L:79:PRO:HD2	1:L:83:GLY:N	1.93	0.83
4:L:282:BCL:HBB2	4:L:282:BCL:HHC	1.60	0.83
3:H:204:HIS:CG	3:H:205:VAL:N	2.47	0.83
1:L:54:VAL:O	1:L:57:GLY:N	2.11	0.83
1:L:113:ILE:CG2	1:L:114:GLY:H	1.90	0.83
3:H:140:PHE:HD2	3:H:169:VAL:HG11	1.41	0.83
1:L:73:TYR:HD2	1:L:82:LYS:CE	1.87	0.83
1:L:97:PHE:HZ	4:L:283:BCL:H122	1.39	0.83
1:L:168:HIS:O	1:L:169:TYR:CD1	2.30	0.83
2:M:18:LEU:HD12	2:M:18:LEU:N	1.93	0.83
1:L:79:PRO:HD2	1:L:83:GLY:H	1.43	0.83
2:M:238:ILE:HD11	2:M:263:GLU:CA	2.08	0.83
2:M:235:LEU:H	2:M:235:LEU:CD1	1.90	0.83
1:L:84:GLY:O	1:L:86:TRP:N	2.10	0.82
1:L:170:ASN:HB2	1:L:259:TRP:NE1	1.93	0.82
2:M:109:LEU:O	2:M:114:LEU:HD13	1.78	0.82
1:L:205:GLU:CA	3:H:65:ILE:CG2	2.57	0.82
2:M:87:ARG:HD2	2:M:88:ASP:OD2	1.76	0.82
1:L:186:ALA:C	2:M:216:PHE:HE2	1.83	0.82
3:H:27:LEU:HD13	3:H:32:GLN:NE2	1.93	0.82
1:L:175:ILE:CG2	1:L:243:PHE:CE2	2.48	0.82
1:L:214:THR:HG22	2:M:140:LEU:CD2	2.08	0.82
5:L:284:BPH:H143	5:L:284:BPH:H171	0.83	0.82
2:M:154:ILE:HG23	2:M:157:TRP:HE3	1.44	0.82
2:M:277:THR:HG23	2:M:277:THR:O	1.78	0.82
3:H:37:ARG:O	3:H:42:LEU:HD11	1.80	0.82
2:M:20:MET:HG3	2:M:21:THR:CA	2.10	0.82
3:H:151:LEU:CD2	3:H:203:VAL:HG23	2.10	0.82
1:L:124:ALA:C	1:L:126:LEU:H	1.81	0.82
1:L:156:TRP:CZ3	1:L:157:VAL:HA	2.15	0.82
1:L:195:LEU:HB3	2:M:145:HIS:HD2	1.41	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:90:PHE:HD2	2:M:180:PHE:CD1	1.96	0.82
2:M:171:TRP:C	2:M:173:GLU:N	2.32	0.82
3:H:123:LEU:CD2	3:H:127:GLY:HA2	2.09	0.82
3:H:143:SER:O	3:H:144:ALA:HB3	1.80	0.82
1:L:24:PHE:O	1:L:31:VAL:HG23	1.78	0.82
1:L:107:ILE:CD1	2:M:255:THR:OG1	2.27	0.82
1:L:234:LEU:HD12	2:M:221:ALA:CA	2.10	0.82
2:M:227:SER:O	2:M:230:GLY:N	2.06	0.82
1:L:33:PHE:CD1	1:L:33:PHE:C	2.50	0.82
2:M:175:VAL:HG22	2:M:185:TRP:CZ2	2.14	0.82
3:H:130:LYS:O	3:H:171:ILE:HD13	1.79	0.82
3:H:147:ASN:O	3:H:151:LEU:HD12	1.79	0.82
2:M:186:THR:O	2:M:189:PHE:HB3	1.80	0.82
3:H:15:LEU:HA	3:H:18:TYR:HD2	1.45	0.82
3:H:134:MET:HE1	3:H:167:ILE:HD12	1.61	0.82
2:M:131:GLY:O	2:M:134:TYR:CA	2.28	0.82
1:L:124:ALA:HB2	5:L:284:BPH:HBC2	1.62	0.81
4:M:310:BCL:CBB	4:M:310:BCL:HHC	2.09	0.81
4:M:310:BCL:HHC	4:M:310:BCL:HBB3	1.62	0.81
1:L:54:VAL:O	1:L:56:GLN:N	2.13	0.81
1:L:156:TRP:O	1:L:156:TRP:CD2	2.34	0.81
1:L:156:TRP:HE3	1:L:157:VAL:CA	1.94	0.81
1:L:185:LEU:O	1:L:187:LEU:N	2.12	0.81
1:L:242:PHE:CD1	1:L:242:PHE:C	2.52	0.81
5:M:312:BPH:C6	5:M:312:BPH:C8	2.58	0.81
3:H:14:SER:O	3:H:18:TYR:CB	2.27	0.81
3:H:17:ILE:O	3:H:17:ILE:HD13	1.81	0.81
1:L:181:PHE:O	1:L:184:ALA:HB3	1.80	0.81
2:M:99:PRO:HG2	2:M:111:GLU:HG3	1.61	0.81
2:M:26:LEU:HD23	2:M:27:ALA:N	1.94	0.81
3:H:134:MET:SD	3:H:141:HIS:ND1	2.54	0.81
3:H:156:CYS:O	3:H:157:ASP:C	2.19	0.81
1:L:232:LEU:CA	2:M:42:PHE:HZ	1.94	0.81
2:M:102:GLY:C	2:M:104:SER:H	1.84	0.81
3:H:185:ASP:O	3:H:187:SER:N	2.14	0.81
1:L:119:PHE:CE1	1:L:238:LEU:HD11	2.16	0.81
1:L:212:GLU:O	1:L:214:THR:N	2.12	0.81
2:M:156:LEU:O	2:M:156:LEU:HD23	1.81	0.81
3:H:56:PHE:O	3:H:58:LEU:N	2.14	0.81
1:L:135:ARG:CG	1:L:139:MET:CE	2.57	0.81
1:L:260:VAL:HG12	1:L:260:VAL:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:LEU:O	2:M:68:PHE:N	2.14	0.81
2:M:65:MET:CG	2:M:66:TRP:N	2.38	0.81
2:M:186:THR:HG23	4:M:310:BCL:CMD	2.04	0.81
2:M:271:TRP:HZ3	3:H:31:LEU:HD23	1.45	0.81
1:L:75:LEU:HG	1:L:140:GLY:O	1.81	0.81
1:L:219:LEU:CA	2:M:132:ARG:HH21	1.93	0.81
1:L:127:ALA:CB	4:L:283:BCL:H2	2.10	0.81
6:L:285:U10:H112	6:L:285:U10:H153	1.62	0.81
2:M:17:ASP:O	2:M:18:LEU:HG	1.81	0.81
2:M:90:PHE:CA	2:M:179:ILE:HD12	2.09	0.81
1:L:22:PHE:HB3	1:L:32:GLY:HA2	1.63	0.80
1:L:219:LEU:O	2:M:132:ARG:NH2	2.14	0.80
1:L:69:PRO:HB3	1:L:78:ALA:CB	2.11	0.80
4:L:283:BCL:H143	5:L:284:BPH:CGA	2.11	0.80
1:L:123:PHE:O	1:L:126:LEU:HB3	1.79	0.80
4:L:282:BCL:H11	5:M:312:BPH:OBB	1.81	0.80
3:H:194:GLN:H	3:H:194:GLN:NE2	1.78	0.80
1:L:195:LEU:HD21	2:M:267:ARG:HD3	1.64	0.80
3:H:60:LYS:HG3	3:H:60:LYS:O	1.81	0.80
3:H:130:LYS:HB3	3:H:130:LYS:HZ3	1.44	0.80
3:H:246:PRO:O	3:H:248:ARG:HG3	1.82	0.80
1:L:132:VAL:O	1:L:132:VAL:HG12	1.80	0.80
1:L:133:LEU:HD12	1:L:137:VAL:HG23	1.64	0.80
1:L:204:LYS:HD2	1:L:207:ARG:HH22	1.47	0.80
1:L:219:LEU:HD21	2:M:133:THR:CG2	2.11	0.80
1:L:224:ILE:CD1	1:L:232:LEU:HD12	2.11	0.80
1:L:156:TRP:CE3	1:L:157:VAL:CA	2.64	0.80
1:L:262:TRP:O	1:L:264:GLN:N	2.15	0.80
3:H:238:ALA:O	3:H:241:LEU:N	2.14	0.80
2:M:108:PRO:CG	2:M:111:GLU:HB3	2.12	0.80
3:H:111:PRO:HD2	3:H:243:TYR:HE1	1.46	0.80
3:H:154:ARG:HE	3:H:160:ILE:HG13	1.45	0.80
1:L:42:ALA:O	1:L:46:ILE:HG23	1.81	0.80
2:M:120:PHE:CD1	2:M:162:PHE:HE2	1.99	0.80
4:L:283:BCL:H43	5:L:284:BPH:CAB	2.11	0.79
2:M:206:ILE:HD13	4:M:311:BCL:HMD1	1.62	0.79
1:L:49:ILE:HG23	1:L:50:ALA:N	1.97	0.79
2:M:35:PHE:CD2	2:M:39:LEU:CD2	2.65	0.79
3:H:196:VAL:HA	3:H:204:HIS:C	2.02	0.79
2:M:196:LEU:HD12	2:M:199:ASN:HB2	1.63	0.79
3:H:117:ARG:HB2	3:H:227:LEU:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:155:GLY:O	3:H:204:HIS:CD2	2.33	0.79
2:M:134:TYR:HD1	2:M:134:TYR:O	1.64	0.79
2:M:205:SER:O	4:M:310:BCL:CMA	2.29	0.79
1:L:58:THR:O	1:L:59:TRP:HB3	1.81	0.79
2:M:90:PHE:CD2	2:M:180:PHE:CD1	2.71	0.79
3:H:90:THR:O	3:H:91:ALA:CB	2.30	0.79
1:L:232:LEU:CG	2:M:42:PHE:HE2	1.96	0.79
2:M:120:PHE:O	2:M:121:PHE:CD1	2.36	0.79
2:M:264:GLY:O	2:M:268:TRP:N	2.16	0.79
3:H:124:ASP:OD1	3:H:125:GLY:CA	2.29	0.79
1:L:47:ILE:HG22	1:L:48:LEU:H	1.45	0.79
5:L:284:BPH:H143	5:L:284:BPH:H172	1.62	0.79
2:M:218:MET:CE	6:M:313:U10:H1M3	2.12	0.79
2:M:227:SER:HB3	3:H:194:GLN:CG	2.12	0.79
3:H:238:ALA:HA	3:H:241:LEU:HD12	1.63	0.79
1:L:102:LEU:CD2	1:L:102:LEU:N	2.46	0.79
2:M:253:ARG:O	2:M:257:GLY:HA2	1.82	0.79
2:M:20:MET:HG3	2:M:21:THR:H	1.48	0.79
2:M:27:ALA:HB1	2:M:51:TYR:HA	1.65	0.79
3:H:111:PRO:HG2	3:H:242:MET:HB2	1.62	0.79
2:M:73:TRP:CG	2:M:114:LEU:CD2	2.65	0.78
1:L:11:VAL:CG1	3:H:87:LEU:HD11	2.13	0.78
1:L:132:VAL:O	1:L:132:VAL:CG1	2.28	0.78
1:L:179:PHE:HB3	1:L:240:ALA:HB2	1.64	0.78
1:L:226:THR:HG22	2:M:232:GLU:HB3	1.65	0.78
1:L:149:GLY:C	1:L:151:TRP:H	1.84	0.78
1:L:242:PHE:HD1	1:L:243:PHE:H	1.29	0.78
2:M:64:LEU:CD1	5:M:312:BPH:C7	2.55	0.78
2:M:99:PRO:CG	2:M:111:GLU:HG3	2.14	0.78
2:M:208:PHE:C	2:M:210:TYR:H	1.86	0.78
3:H:127:GLY:O	3:H:129:ASN:N	2.17	0.78
1:L:101:ALA:O	1:L:104:GLU:HB2	1.83	0.78
1:L:116:HIS:HE1	2:M:225:ALA:HA	1.48	0.78
1:L:205:GLU:CA	3:H:65:ILE:HG21	2.13	0.78
2:M:38:LEU:O	2:M:40:GLY:N	2.16	0.78
2:M:114:LEU:CD1	2:M:114:LEU:N	2.41	0.78
2:M:212:SER:O	2:M:213:ALA:C	2.20	0.78
2:M:222:THR:O	2:M:225:ALA:N	2.14	0.78
2:M:290:VAL:O	2:M:290:VAL:HG12	1.84	0.78
3:H:13:ALA:O	3:H:16:ALA:HB3	1.83	0.78
3:H:201:ASN:OD1	3:H:202:ARG:N	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:PRO:HG3	1:L:83:GLY:CA	2.13	0.78
1:L:173:HIS:HB2	1:L:247:CYS:SG	2.23	0.78
1:L:183:ASN:C	1:L:183:ASN:HD22	1.85	0.78
1:L:225:GLY:HA3	3:H:173:GLU:OE2	1.84	0.78
2:M:284:ILE:HG13	4:M:310:BCL:HED1	1.64	0.78
1:L:93:ALA:HB3	1:L:128:TYR:OH	1.84	0.78
1:L:135:ARG:HB3	1:L:136:PRO:CD	2.09	0.78
1:L:185:LEU:C	1:L:187:LEU:N	2.33	0.78
2:M:17:ASP:HA	2:M:18:LEU:HD12	1.65	0.78
2:M:89:LEU:HA	2:M:92:PHE:HD2	1.46	0.78
2:M:241:ARG:CB	2:M:241:ARG:NH1	2.47	0.78
2:M:296:VAL:O	2:M:297:TRP:C	2.22	0.78
3:H:111:PRO:HG2	3:H:242:MET:CG	2.12	0.78
3:H:234:CYS:O	3:H:237:VAL:HG23	1.83	0.78
1:L:53:ALA:CB	1:L:64:ILE:HG12	2.13	0.78
1:L:92:CYS:O	1:L:96:ALA:HB2	1.83	0.78
3:H:184:LYS:HA	3:H:184:LYS:CE	2.14	0.78
3:H:207:ALA:O	3:H:247:LYS:NZ	2.14	0.78
1:L:25:TRP:CH2	1:L:110:LYS:NZ	2.51	0.78
1:L:177:ILE:HD13	4:L:283:BCL:HHB	1.65	0.78
2:M:119:SER:HB2	2:M:177:TYR:OH	1.84	0.78
2:M:126:VAL:CG1	2:M:154:ILE:CD1	2.62	0.78
1:L:127:ALA:HB1	4:L:283:BCL:H2	1.67	0.78
4:L:283:BCL:C2C	4:M:310:BCL:HBC2	2.13	0.78
4:L:283:BCL:CBD	4:M:311:BCL:HBC1	2.14	0.78
3:H:42:LEU:CD2	3:H:77:GLY:H	1.97	0.78
3:H:103:ASP:HB3	3:H:106:LYS:HE3	1.66	0.78
3:H:182:GLU:HA	3:H:187:SER:O	1.84	0.78
1:L:24:PHE:CZ	1:L:31:VAL:HG21	2.19	0.77
1:L:48:LEU:HD11	1:L:89:ILE:CG1	2.14	0.77
1:L:180:PHE:HE1	2:M:213:ALA:CB	1.97	0.77
3:H:12:LEU:HD23	3:H:12:LEU:O	1.83	0.77
3:H:117:ARG:HB2	3:H:227:LEU:HB3	1.65	0.77
3:H:148:PRO:O	3:H:151:LEU:CB	2.32	0.77
3:H:183:LEU:HD21	3:H:189:ARG:HG2	1.66	0.77
1:L:224:ILE:O	1:L:224:ILE:HG22	1.84	0.77
1:L:182:THR:C	1:L:184:ALA:H	1.87	0.77
1:L:263:TRP:CD1	2:M:180:PHE:HE2	2.01	0.77
2:M:243:THR:HG21	2:M:247:ARG:NH2	1.99	0.77
3:H:191:LEU:HD23	3:H:213:PHE:CE1	2.20	0.77
3:H:132:LYS:HZ2	3:H:223:THR:CG2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:LEU:HD12	1:L:89:ILE:CD1	2.14	0.77
1:L:156:TRP:CE3	1:L:157:VAL:N	2.51	0.77
1:L:182:THR:O	1:L:185:LEU:HD21	1.83	0.77
1:L:269:LEU:HB3	1:L:270:PRO:CD	2.11	0.77
1:L:269:LEU:CG	1:L:270:PRO:CD	2.62	0.77
1:L:25:TRP:O	1:L:27:GLY:N	2.18	0.77
1:L:31:VAL:HG12	1:L:36:VAL:CG2	2.15	0.77
1:L:46:ILE:HA	1:L:49:ILE:CG2	2.14	0.77
1:L:153:HIS:HD2	1:L:154:LEU:CD1	1.98	0.77
1:L:175:ILE:HD13	1:L:243:PHE:HE2	0.65	0.77
2:M:197:PHE:HE1	4:M:311:BCL:HMD1	1.50	0.77
3:H:157:ASP:OD1	3:H:210:SER:N	2.18	0.77
2:M:204:LEU:O	2:M:207:ALA:CB	2.33	0.77
1:L:111:LEU:CD2	2:M:251:PHE:HB2	2.14	0.77
5:M:312:BPH:HHD	5:M:312:BPH:CBC	2.12	0.77
3:H:111:PRO:CG	3:H:242:MET:CG	2.63	0.77
2:M:93:SER:HB2	2:M:178:GLY:HA3	1.67	0.76
2:M:98:ALA:HA	2:M:99:PRO:C	2.04	0.76
2:M:209:LEU:N	2:M:276:VAL:CG2	2.47	0.76
3:H:44:ASN:ND2	3:H:44:ASN:N	2.29	0.76
3:H:52:ASN:O	3:H:53:GLN:HB2	1.83	0.76
5:L:284:BPH:H171	5:L:284:BPH:H141	1.61	0.76
2:M:119:SER:CA	2:M:177:TYR:OH	2.33	0.76
3:H:108:GLY:HA3	3:H:114:TRP:CZ3	2.20	0.76
1:L:21:LEU:CD1	1:L:22:PHE:HE1	1.95	0.76
2:M:11:GLN:HB3	3:H:143:SER:O	1.85	0.76
3:H:12:LEU:CD2	3:H:13:ALA:N	2.48	0.76
1:L:73:TYR:CE2	1:L:82:LYS:HE3	2.20	0.76
2:M:196:LEU:HD11	2:M:199:ASN:ND2	2.01	0.76
1:L:73:TYR:CB	1:L:82:LYS:NZ	2.46	0.76
3:H:195:MET:C	3:H:196:VAL:CG1	2.51	0.76
1:L:46:ILE:O	1:L:46:ILE:HG13	1.85	0.76
1:L:69:PRO:CG	1:L:78:ALA:HB3	2.16	0.76
1:L:133:LEU:HD12	1:L:137:VAL:CG2	2.15	0.76
1:L:151:TRP:CE3	1:L:154:LEU:HD22	2.20	0.76
1:L:154:LEU:HD12	1:L:154:LEU:N	2.00	0.76
3:H:215:GLY:HA3	3:H:236:TYR:OH	1.84	0.76
1:L:5:PHE:HZ	3:H:40:TYR:CZ	2.02	0.76
2:M:205:SER:O	4:M:310:BCL:HMA2	1.85	0.76
2:M:236:GLU:CG	3:H:122:GLU:HG3	2.16	0.76
1:L:7:ARG:O	3:H:87:LEU:CD2	2.28	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:118:ALA:O	2:M:121:PHE:N	2.19	0.76
3:H:90:THR:O	3:H:91:ALA:HB2	1.86	0.76
3:H:124:ASP:O	3:H:126:HIS:N	2.18	0.76
1:L:22:PHE:CE2	1:L:36:VAL:HG11	2.17	0.76
1:L:49:ILE:CA	1:L:89:ILE:HD11	2.16	0.76
1:L:60:ASN:C	1:L:62:GLN:N	2.35	0.76
1:L:263:TRP:CD1	2:M:180:PHE:CE2	2.74	0.76
5:L:284:BPH:C17	5:L:284:BPH:H141	2.15	0.76
1:L:12:PRO:HD3	3:H:97:PRO:HB2	1.66	0.76
1:L:108:CYS:O	1:L:109:ARG:C	2.25	0.76
1:L:185:LEU:CD2	1:L:186:ALA:N	2.18	0.75
1:L:248:MET:O	1:L:249:ILE:C	2.23	0.75
2:M:264:GLY:O	2:M:267:ARG:HB2	1.86	0.75
1:L:43:ALA:C	1:L:45:GLY:H	1.89	0.75
1:L:208:THR:H	1:L:211:HIS:CG	2.04	0.75
6:L:285:U10:H303	6:L:285:U10:C26	2.15	0.75
1:L:180:PHE:CE1	2:M:213:ALA:HB2	2.19	0.75
4:L:283:BCL:H141	5:L:284:BPH:O2A	1.86	0.75
2:M:20:MET:SD	2:M:22:GLU:N	2.59	0.75
2:M:163:ILE:HG21	2:M:285:LEU:HD13	1.68	0.75
2:M:196:LEU:CD1	2:M:199:ASN:HB2	2.16	0.75
1:L:8:LYS:CA	3:H:87:LEU:CD2	2.54	0.75
1:L:94:THR:CB	1:L:129:LEU:HD11	2.15	0.75
1:L:175:ILE:HG22	1:L:176:ALA:N	2.00	0.75
1:L:219:LEU:CD2	2:M:133:THR:HG23	2.14	0.75
4:L:283:BCL:C14	5:L:284:BPH:CBA	2.60	0.75
2:M:194:GLY:O	2:M:195:ASN:C	2.24	0.75
2:M:264:GLY:CA	2:M:267:ARG:HB2	2.17	0.75
3:H:142:VAL:O	3:H:142:VAL:HG12	1.87	0.75
3:H:148:PRO:C	3:H:151:LEU:HB2	2.06	0.75
1:L:112:GLY:O	1:L:113:ILE:O	2.05	0.75
1:L:113:ILE:CD1	2:M:226:VAL:HG22	2.16	0.75
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.68	0.75
1:L:197:ALA:HB1	2:M:235:LEU:HD21	1.69	0.75
1:L:15:THR:HG21	1:L:19:GLY:CA	2.16	0.75
4:L:283:BCL:H112	5:L:284:BPH:HBA2	1.69	0.75
2:M:25:ASN:O	2:M:27:ALA:O	2.05	0.75
1:L:206:MET:H	3:H:65:ILE:HG22	0.69	0.75
1:L:226:THR:HG23	2:M:232:GLU:O	1.86	0.75
2:M:81:ASN:O	2:M:84:VAL:HB	1.85	0.75
6:L:285:U10:O4	6:L:285:U10:C3M	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:46:GLN:CG	2:M:47:LEU:N	2.46	0.75
2:M:71:GLY:O	2:M:74:PHE:CB	2.35	0.75
1:L:60:ASN:O	1:L:63:LEU:N	2.18	0.75
1:L:133:LEU:O	1:L:137:VAL:CG2	2.32	0.75
2:M:78:ALA:O	2:M:84:VAL:HG11	1.86	0.75
3:H:219:ILE:HG23	3:H:229:GLU:HG2	1.66	0.75
1:L:171:PRO:O	1:L:174:MET:N	2.19	0.74
1:L:177:ILE:HD13	4:L:283:BCL:CHB	2.16	0.74
1:L:182:THR:O	1:L:184:ALA:N	2.20	0.74
2:M:21:THR:CB	2:M:139:ALA:HB1	2.10	0.74
2:M:20:MET:HG3	2:M:22:GLU:H	1.52	0.74
2:M:88:ASP:CA	2:M:92:PHE:CZ	2.70	0.74
3:H:27:LEU:HD11	3:H:28:ILE:HG13	1.68	0.74
3:H:92:VAL:CG1	3:H:93:SER:H	2.01	0.74
1:L:151:TRP:CZ3	1:L:154:LEU:CD2	2.70	0.74
2:M:13:ARG:NH1	2:M:34:PRO:HB3	2.01	0.74
2:M:291:VAL:HG13	2:M:293:ASN:O	1.87	0.74
2:M:12:VAL:C	2:M:13:ARG:HG2	2.07	0.74
2:M:289:THR:C	2:M:291:VAL:H	1.89	0.74
4:M:311:BCL:HMB1	4:M:311:BCL:HBB2	1.69	0.74
3:H:120:LEU:HD23	3:H:121:PRO:O	1.88	0.74
1:L:94:THR:OG1	1:L:129:LEU:HD12	1.86	0.74
2:M:135:LEU:CB	2:M:138:GLN:OE1	2.36	0.74
3:H:36:MET:CE	3:H:36:MET:CA	2.61	0.74
3:H:134:MET:CE	3:H:167:ILE:HB	2.15	0.74
1:L:39:PHE:C	1:L:41:PHE:H	1.91	0.74
1:L:146:PHE:HB3	1:L:156:TRP:NE1	2.02	0.74
1:L:226:THR:HG22	2:M:232:GLU:CB	2.17	0.74
2:M:25:ASN:O	2:M:26:LEU:C	2.24	0.74
1:L:51:TRP:CH2	1:L:80:LEU:HD13	2.23	0.74
1:L:146:PHE:HB3	1:L:156:TRP:CD1	2.21	0.74
1:L:170:ASN:HB2	1:L:259:TRP:CE2	2.22	0.74
2:M:114:LEU:O	2:M:117:ILE:CB	2.32	0.74
2:M:205:SER:CB	2:M:279:THR:HG22	2.16	0.74
1:L:123:PHE:CG	1:L:238:LEU:HD21	2.22	0.74
2:M:46:GLN:HE21	2:M:49:PRO:HD2	1.53	0.74
2:M:208:PHE:O	2:M:210:TYR:N	2.21	0.74
2:M:284:ILE:HD12	4:M:310:BCL:CED	2.17	0.74
3:H:133:PRO:HA	3:H:168:TRP:HA	1.68	0.74
3:H:228:LEU:O	3:H:232:LYS:HB2	1.87	0.74
1:L:6:GLU:HG2	1:L:10:ARG:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:GLY:O	1:L:99:SER:HB3	1.87	0.74
6:L:285:U10:O4	6:L:285:U10:H3M3	1.87	0.74
3:H:14:SER:O	3:H:18:TYR:CD2	2.41	0.74
1:L:255:TRP:HZ2	1:L:262:TRP:N	1.86	0.73
2:M:85:PHE:CE1	2:M:89:LEU:CD1	2.71	0.73
2:M:206:ILE:CD1	4:M:310:BCL:C1B	2.64	0.73
3:H:116:ALA:CA	3:H:228:LEU:CD1	2.65	0.73
3:H:124:ASP:OD1	3:H:126:HIS:N	2.19	0.73
3:H:130:LYS:HB3	3:H:130:LYS:NZ	1.99	0.73
3:H:148:PRO:HA	3:H:151:LEU:CD1	2.17	0.73
1:L:135:ARG:NH1	1:L:139:MET:HE1	2.01	0.73
1:L:197:ALA:HB1	2:M:235:LEU:CD2	2.16	0.73
1:L:222:TYR:O	1:L:223:SER:CB	2.36	0.73
2:M:114:LEU:H	2:M:114:LEU:HD13	1.50	0.73
3:H:82:ASP:O	3:H:84:PRO:CD	2.36	0.73
3:H:198:VAL:O	3:H:198:VAL:HG12	1.86	0.73
1:L:102:LEU:HD23	1:L:102:LEU:N	2.00	0.73
1:L:113:ILE:CG2	1:L:114:GLY:N	2.51	0.73
1:L:171:PRO:O	1:L:174:MET:HB2	1.88	0.73
2:M:35:PHE:HD1	2:M:38:LEU:HB2	1.47	0.73
2:M:146:THR:O	2:M:150:PHE:HB2	1.87	0.73
1:L:232:LEU:O	1:L:235:LEU:CB	2.37	0.73
2:M:58:LEU:HA	2:M:61:PHE:HB3	1.70	0.73
2:M:128:SER:O	2:M:131:GLY:N	2.21	0.73
1:L:241:VAL:CG1	1:L:242:PHE:N	2.51	0.73
1:L:269:LEU:HD22	1:L:270:PRO:HD3	0.78	0.73
2:M:46:GLN:HG2	2:M:48:GLY:O	1.88	0.73
2:M:75:TRP:O	2:M:78:ALA:N	2.20	0.73
2:M:284:ILE:CD1	4:M:310:BCL:O2D	2.36	0.73
3:H:92:VAL:HG12	3:H:93:SER:H	1.54	0.73
3:H:226:THR:HG22	3:H:229:GLU:CD	2.09	0.73
2:M:215:LEU:O	2:M:215:LEU:HD12	1.88	0.73
3:H:19:SER:O	3:H:20:PHE:C	2.27	0.73
1:L:123:PHE:O	1:L:126:LEU:CB	2.36	0.73
1:L:225:GLY:HA2	6:L:285:U10:C4M	2.17	0.73
1:L:244:SER:HB3	4:L:283:BCL:HED3	1.71	0.73
2:M:185:TRP:O	2:M:185:TRP:CG	2.41	0.73
2:M:271:TRP:O	2:M:274:VAL:N	2.22	0.73
3:H:114:TRP:CD1	3:H:115:VAL:O	2.42	0.73
2:M:152:SER:CB	2:M:277:THR:HG22	2.19	0.73
1:L:259:TRP:O	1:L:261:ASP:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:THR:CG2	2:M:38:LEU:N	2.51	0.72
2:M:67:PHE:HD1	2:M:68:PHE:N	1.87	0.72
2:M:113:GLY:O	2:M:114:LEU:C	2.26	0.72
1:L:133:LEU:N	1:L:136:PRO:HG2	2.04	0.72
1:L:204:LYS:HB3	1:L:207:ARG:NH1	2.01	0.72
1:L:205:GLU:O	1:L:207:ARG:NH1	2.21	0.72
2:M:268:TRP:NE1	6:M:313:U10:H111	2.05	0.72
2:M:87:ARG:CD	2:M:88:ASP:OD2	2.34	0.72
2:M:237:GLN:HG2	2:M:240:ASP:O	1.89	0.72
1:L:151:TRP:CZ3	2:M:198:TYR:HD1	2.08	0.72
4:M:311:BCL:HMB1	4:M:311:BCL:HBB3	1.68	0.72
3:H:134:MET:CE	3:H:141:HIS:CE1	2.73	0.72
3:H:168:TRP:N	3:H:178:PHE:O	2.22	0.72
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.52	0.72
2:M:28:ASN:C	2:M:29:ARG:O	2.24	0.72
2:M:90:PHE:CG	2:M:179:ILE:HD12	2.24	0.72
2:M:96:PRO:CB	2:M:97:PRO:CD	2.58	0.72
2:M:109:LEU:C	2:M:109:LEU:CD2	2.57	0.72
3:H:37:ARG:O	3:H:42:LEU:CD1	2.36	0.72
1:L:84:GLY:C	1:L:86:TRP:N	2.41	0.72
1:L:97:PHE:CE1	4:L:283:BCL:C11	2.73	0.72
2:M:54:SER:C	2:M:57:VAL:HG13	2.07	0.72
2:M:241:ARG:HH12	2:M:246:GLU:CG	2.02	0.72
3:H:30:TYR:O	3:H:34:GLU:HB2	1.90	0.72
1:L:48:LEU:HD12	1:L:89:ILE:HD12	1.69	0.72
2:M:20:MET:CG	2:M:22:GLU:H	2.02	0.72
2:M:126:VAL:HG12	2:M:154:ILE:HD11	1.72	0.72
2:M:266:HIS:O	2:M:270:ILE:HG22	1.90	0.72
3:H:111:PRO:HD2	3:H:243:TYR:CZ	2.25	0.72
1:L:113:ILE:CD1	2:M:226:VAL:CG2	2.68	0.72
1:L:114:GLY:H	2:M:225:ALA:HB1	1.55	0.72
1:L:167:PHE:CZ	1:L:251:THR:HG21	2.25	0.72
2:M:245:ALA:O	2:M:247:ARG:N	2.23	0.72
7:M:308:BOG:O2	7:M:308:BOG:C5	2.37	0.72
3:H:194:GLN:N	3:H:194:GLN:OE1	2.22	0.72
1:L:185:LEU:HB3	5:M:312:BPH:H3C	1.71	0.72
5:M:312:BPH:HBC3	5:M:312:BPH:CHD	2.16	0.72
3:H:40:TYR:N	3:H:42:LEU:CD1	2.53	0.72
1:L:113:ILE:HG23	1:L:114:GLY:H	1.55	0.72
2:M:73:TRP:CE2	2:M:114:LEU:HG	2.24	0.72
2:M:260:ALA:HA	3:H:36:MET:HG3	0.81	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:313:U10:C8	6:M:313:U10:H1M1	2.20	0.72
1:L:113:ILE:HD12	2:M:226:VAL:HG23	1.71	0.71
1:L:187:LEU:CD2	2:M:216:PHE:CG	2.73	0.71
2:M:9:GLN:HE22	3:H:197:LYS:HD2	1.54	0.71
3:H:14:SER:O	3:H:18:TYR:HD2	1.73	0.71
3:H:133:PRO:HD2	3:H:136:ALA:CB	2.20	0.71
1:L:6:GLU:HG2	1:L:10:ARG:CG	2.19	0.71
1:L:53:ALA:CA	1:L:64:ILE:HD13	2.20	0.71
1:L:116:HIS:HE1	2:M:225:ALA:CA	2.04	0.71
4:L:283:BCL:C14	5:L:284:BPH:CGA	2.68	0.71
2:M:25:ASN:O	2:M:27:ALA:N	2.23	0.71
2:M:71:GLY:O	2:M:74:PHE:HB3	1.90	0.71
2:M:291:VAL:HG21	2:M:294:TRP:CH2	2.25	0.71
1:L:102:LEU:H	1:L:102:LEU:CD2	1.99	0.71
4:L:283:BCL:H151	5:L:284:BPH:C3A	2.17	0.71
2:M:136:ARG:NE	2:M:136:ARG:CA	2.53	0.71
2:M:154:ILE:HG23	2:M:157:TRP:CE3	2.23	0.71
2:M:170:SER:OG	2:M:172:SER:HB3	1.91	0.71
3:H:204:HIS:NE2	3:H:205:VAL:O	2.23	0.71
1:L:75:LEU:HD21	1:L:141:ALA:C	2.11	0.71
1:L:119:PHE:O	1:L:122:ALA:HB3	1.90	0.71
1:L:146:PHE:HB2	1:L:147:PRO:CD	2.20	0.71
1:L:193:LEU:HG	1:L:212:GLU:OE1	1.90	0.71
2:M:136:ARG:HA	2:M:136:ARG:NE	2.04	0.71
2:M:205:SER:N	2:M:279:THR:HG21	2.05	0.71
2:M:39:LEU:H	2:M:39:LEU:HD22	1.55	0.71
3:H:40:TYR:N	3:H:42:LEU:HD13	2.05	0.71
3:H:26:GLY:O	3:H:30:TYR:HB2	1.90	0.71
3:H:246:PRO:O	3:H:248:ARG:CG	2.38	0.71
2:M:21:THR:HG22	2:M:140:LEU:CD1	2.21	0.71
2:M:186:THR:O	2:M:189:PHE:CB	2.38	0.71
3:H:59:PRO:O	3:H:61:PRO:HD3	1.89	0.71
3:H:116:ALA:CB	3:H:228:LEU:HD11	2.21	0.71
2:M:35:PHE:CG	2:M:39:LEU:HD22	2.26	0.71
3:H:128:HIS:C	3:H:130:LYS:H	1.94	0.71
1:L:16:LEU:HB3	1:L:106:GLU:OE2	1.91	0.71
1:L:146:PHE:O	1:L:147:PRO:O	2.07	0.71
3:H:20:PHE:CZ	3:H:24:LEU:CD1	2.68	0.71
3:H:157:ASP:O	3:H:158:LEU:HB2	1.88	0.71
3:H:124:ASP:CG	3:H:125:GLY:N	2.42	0.71
3:H:148:PRO:O	3:H:164:VAL:CG2	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:218:THR:HG22	3:H:219:ILE:O	1.91	0.71
1:L:47:ILE:HG22	1:L:48:LEU:N	2.06	0.70
6:L:285:U10:H152	6:L:285:U10:H111	0.73	0.70
1:L:72:GLU:OE2	1:L:73:TYR:N	2.23	0.70
1:L:171:PRO:HA	1:L:174:MET:CG	2.21	0.70
2:M:35:PHE:CE1	2:M:38:LEU:HD13	2.25	0.70
2:M:218:MET:HE2	6:M:313:U10:H1M3	1.73	0.70
2:M:37:THR:HG22	2:M:38:LEU:N	2.07	0.70
2:M:73:TRP:CE2	2:M:114:LEU:CD1	2.75	0.70
2:M:153:ALA:O	4:M:310:BCL:H71	1.91	0.70
2:M:206:ILE:HD11	4:M:310:BCL:C2B	2.21	0.70
3:H:92:VAL:CG1	3:H:93:SER:N	2.54	0.70
2:M:64:LEU:O	2:M:67:PHE:N	2.24	0.70
2:M:139:ALA:HB3	2:M:140:LEU:CD1	2.21	0.70
2:M:149:ALA:HB2	2:M:270:ILE:HD12	1.74	0.70
3:H:12:LEU:O	3:H:14:SER:N	2.24	0.70
3:H:82:ASP:O	3:H:84:PRO:HD2	1.92	0.70
3:H:146:LYS:NZ	3:H:198:VAL:HG12	2.06	0.70
1:L:177:ILE:CD1	4:L:283:BCL:C1B	2.70	0.70
1:L:231:ARG:O	1:L:235:LEU:HD23	1.92	0.70
2:M:156:LEU:HG	2:M:160:LEU:HD22	1.73	0.70
1:L:147:PRO:O	1:L:148:TYR:CD1	2.43	0.70
1:L:224:ILE:HD12	1:L:232:LEU:CD1	2.19	0.70
2:M:196:LEU:HD13	2:M:294:TRP:HD1	1.52	0.70
2:M:206:ILE:HD13	4:M:311:BCL:CMD	2.21	0.70
1:L:128:TYR:O	1:L:129:LEU:C	2.29	0.70
2:M:156:LEU:HD21	2:M:160:LEU:HD23	1.72	0.70
3:H:183:LEU:HD21	3:H:189:ARG:CG	2.21	0.70
1:L:149:GLY:C	1:L:151:TRP:N	2.39	0.70
2:M:51:TYR:CD1	2:M:51:TYR:C	2.63	0.70
2:M:73:TRP:CG	2:M:114:LEU:CG	2.71	0.70
2:M:73:TRP:CE2	2:M:114:LEU:HD11	2.25	0.70
2:M:156:LEU:O	2:M:160:LEU:HB2	1.92	0.70
2:M:203:GLY:HA2	4:M:311:BCL:OBD	1.92	0.70
3:H:22:ILE:O	3:H:24:LEU:N	2.24	0.70
3:H:229:GLU:C	3:H:233:ILE:HG12	2.11	0.70
1:L:97:PHE:CE1	4:L:283:BCL:C12	2.75	0.70
4:L:283:BCL:HMC2	4:M:310:BCL:HBC1	1.66	0.70
2:M:33:GLY:O	2:M:34:PRO:C	2.28	0.70
2:M:109:LEU:HA	2:M:113:GLY:HA3	1.73	0.70
3:H:134:MET:CE	3:H:141:HIS:HE1	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ALA:CB	1:L:64:ILE:HB	2.22	0.69
1:L:69:PRO:HG3	1:L:83:GLY:HA2	1.74	0.69
1:L:248:MET:HE1	4:L:283:BCL:CAD	2.21	0.69
1:L:248:MET:HE1	4:L:283:BCL:CMD	2.22	0.69
2:M:39:LEU:N	2:M:39:LEU:CD1	2.45	0.69
2:M:109:LEU:HD22	2:M:110:LYS:CA	2.22	0.69
3:H:93:SER:O	3:H:96:PHE:HB2	1.92	0.69
1:L:183:ASN:HB2	1:L:236:LEU:CB	2.20	0.69
2:M:46:GLN:HE22	2:M:49:PRO:CD	1.95	0.69
1:L:69:PRO:CG	1:L:87:GLN:OE1	2.39	0.69
1:L:208:THR:H	1:L:211:HIS:CD2	2.10	0.69
2:M:139:ALA:HB3	2:M:140:LEU:HD13	1.74	0.69
3:H:168:TRP:CE2	3:H:190:LEU:HD13	2.27	0.69
2:M:299:GLN:NE2	2:M:299:GLN:CA	2.37	0.69
1:L:11:VAL:HG13	3:H:87:LEU:HD21	1.73	0.69
1:L:69:PRO:HG3	1:L:83:GLY:HA3	1.74	0.69
1:L:269:LEU:CD1	1:L:270:PRO:HD2	2.23	0.69
2:M:48:GLY:HA2	2:M:49:PRO:O	1.91	0.69
2:M:241:ARG:NH1	2:M:241:ARG:HB2	2.07	0.69
3:H:48:THR:HG23	3:H:51:ALA:O	1.92	0.69
3:H:226:THR:HG22	3:H:229:GLU:OE1	1.92	0.69
1:L:108:CYS:O	1:L:111:LEU:N	2.24	0.69
2:M:97:PRO:CA	2:M:111:GLU:OE2	2.40	0.69
1:L:165:GLY:HA3	1:L:258:GLN:HG2	1.74	0.69
2:M:197:PHE:HE1	4:M:311:BCL:HMD3	1.57	0.69
3:H:111:PRO:CG	3:H:242:MET:HB2	2.20	0.69
3:H:191:LEU:CD2	3:H:205:VAL:HG11	2.21	0.69
3:H:210:SER:HA	3:H:213:PHE:HD2	1.57	0.69
3:H:215:GLY:HA3	3:H:236:TYR:CE2	2.26	0.69
1:L:25:TRP:HZ2	1:L:110:LYS:HE3	1.57	0.69
1:L:35:GLY:HA2	1:L:38:THR:HB	1.75	0.69
1:L:71:LEU:C	1:L:73:TYR:H	1.96	0.69
1:L:177:ILE:HD12	4:L:283:BCL:C2B	2.23	0.69
1:L:195:LEU:CB	2:M:145:HIS:HD2	2.04	0.69
1:L:231:ARG:NH2	2:M:7:PHE:CA	2.50	0.69
2:M:135:LEU:H	2:M:135:LEU:CD1	1.96	0.69
2:M:206:ILE:CG1	4:M:310:BCL:CHB	2.71	0.69
2:M:208:PHE:CB	2:M:276:VAL:HG23	2.23	0.69
1:L:208:THR:OG1	1:L:211:HIS:CD2	2.46	0.69
2:M:94:LEU:N	2:M:177:TYR:O	2.22	0.69
2:M:121:PHE:O	2:M:123:PHE:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:197:PHE:CE1	4:M:311:BCL:HMD3	2.28	0.69
3:H:27:LEU:HD12	3:H:27:LEU:C	2.09	0.69
3:H:111:PRO:HB2	3:H:239:GLY:HA2	1.74	0.69
3:H:238:ALA:O	3:H:239:GLY:C	2.31	0.69
4:L:283:BCL:HMC2	4:M:310:BCL:HBC2	1.69	0.68
3:H:179:LEU:CD2	3:H:181:VAL:CG2	2.71	0.68
1:L:156:TRP:C	1:L:156:TRP:CD2	2.64	0.68
3:H:85:ILE:C	3:H:87:LEU:H	1.93	0.68
3:H:151:LEU:HD22	3:H:203:VAL:HG22	1.73	0.68
3:H:190:LEU:H	3:H:190:LEU:CD2	2.04	0.68
2:M:88:ASP:C	2:M:92:PHE:CD2	2.67	0.68
3:H:63:THR:HG23	3:H:74:THR:CG2	2.23	0.68
3:H:156:CYS:O	3:H:158:LEU:HD22	1.94	0.68
1:L:45:GLY:O	1:L:49:ILE:HB	1.93	0.68
2:M:21:THR:OG1	2:M:21:THR:O	2.09	0.68
4:M:310:BCL:C4	5:M:312:BPH:HBB2	2.24	0.68
3:H:12:LEU:C	3:H:14:SER:H	1.95	0.68
3:H:27:LEU:CD1	3:H:32:GLN:NE2	2.56	0.68
1:L:10:ARG:HH22	1:L:25:TRP:HB2	1.56	0.68
2:M:20:MET:HG3	2:M:22:GLU:N	2.08	0.68
2:M:291:VAL:HG11	2:M:294:TRP:CE2	2.28	0.68
3:H:35:ASN:HD22	3:H:35:ASN:N	1.92	0.68
3:H:156:CYS:O	3:H:158:LEU:N	2.27	0.68
3:H:207:ALA:C	3:H:247:LYS:HZ1	1.96	0.68
2:M:73:TRP:NE1	2:M:114:LEU:CD1	2.57	0.68
2:M:126:VAL:HG12	2:M:154:ILE:CD1	2.23	0.68
2:M:164:ARG:NH2	2:M:168:MET:HE2	2.09	0.68
2:M:247:ARG:HA	2:M:250:LEU:HB2	1.75	0.68
1:L:73:TYR:HD2	1:L:82:LYS:NZ	1.91	0.68
1:L:86:TRP:O	1:L:87:GLN:C	2.31	0.68
2:M:204:LEU:HA	2:M:207:ALA:HB3	1.75	0.68
1:L:173:HIS:O	1:L:174:MET:C	2.33	0.68
2:M:73:TRP:CD1	2:M:114:LEU:CD2	2.77	0.68
2:M:81:ASN:CG	2:M:84:VAL:CG2	2.63	0.68
2:M:98:ALA:HB2	2:M:172:SER:HA	1.75	0.68
2:M:185:TRP:CD2	2:M:185:TRP:C	2.64	0.68
2:M:214:LEU:O	2:M:217:ALA:CB	2.37	0.68
1:L:101:ALA:HB2	1:L:121:PHE:HE1	1.59	0.67
1:L:107:ILE:HG22	2:M:254:TRP:HE3	1.59	0.67
1:L:153:HIS:CD2	1:L:154:LEU:CD1	2.75	0.67
1:L:167:PHE:CD2	4:L:283:BCL:CHD	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:PRO:O	1:L:172:ALA:C	2.33	0.67
1:L:232:LEU:HA	2:M:42:PHE:CZ	2.23	0.67
1:L:269:LEU:HD13	1:L:270:PRO:HD2	1.76	0.67
2:M:38:LEU:C	2:M:40:GLY:H	1.96	0.67
2:M:192:VAL:HG12	2:M:193:HIS:NE2	2.09	0.67
3:H:12:LEU:HD23	3:H:13:ALA:N	2.08	0.67
1:L:208:THR:O	1:L:211:HIS:CB	2.31	0.67
5:L:284:BPH:C17	5:L:284:BPH:C14	2.11	0.67
2:M:122:MET:O	2:M:122:MET:CG	2.40	0.67
2:M:164:ARG:O	2:M:167:LEU:HB2	1.94	0.67
1:L:103:ARG:HG2	1:L:103:ARG:NH1	2.02	0.67
1:L:182:THR:HG22	1:L:183:ASN:N	2.10	0.67
2:M:35:PHE:CE2	2:M:47:LEU:HD11	2.29	0.67
2:M:132:ARG:O	2:M:134:TYR:N	2.28	0.67
3:H:206:ASN:O	3:H:208:LEU:N	2.28	0.67
1:L:17:VAL:O	1:L:19:GLY:N	2.28	0.67
1:L:144:TYR:C	1:L:145:ALA:O	2.27	0.67
2:M:90:PHE:HA	2:M:179:ILE:CD1	2.18	0.67
2:M:187:ASN:C	2:M:190:SER:H	1.97	0.67
2:M:171:TRP:O	2:M:173:GLU:N	2.28	0.67
3:H:219:ILE:HG22	3:H:229:GLU:OE2	1.92	0.67
1:L:233:GLY:C	1:L:235:LEU:H	1.96	0.67
2:M:152:SER:CA	2:M:277:THR:CG2	2.72	0.67
3:H:103:ASP:C	3:H:106:LYS:HZ1	1.98	0.67
1:L:35:GLY:HA3	6:M:313:U10:H402	1.77	0.67
1:L:202:LYS:HG2	1:L:202:LYS:O	1.94	0.67
1:L:248:MET:CE	4:L:283:BCL:CMD	2.73	0.67
2:M:284:ILE:CG1	4:M:310:BCL:HED1	2.25	0.67
1:L:174:MET:CE	2:M:180:PHE:CZ	2.78	0.67
2:M:89:LEU:N	2:M:92:PHE:HE2	1.93	0.67
2:M:119:SER:CB	2:M:177:TYR:OH	2.43	0.67
2:M:264:GLY:HA2	2:M:267:ARG:CB	2.25	0.67
3:H:80:SER:O	3:H:81:GLU:HG3	1.95	0.67
2:M:39:LEU:H	2:M:39:LEU:CD1	1.97	0.66
6:M:313:U10:H1M1	6:M:313:U10:H8	1.77	0.66
3:H:44:ASN:HD22	3:H:44:ASN:H	1.42	0.66
3:H:146:LYS:NZ	3:H:198:VAL:O	2.28	0.66
1:L:181:PHE:O	1:L:184:ALA:CB	2.43	0.66
2:M:54:SER:O	2:M:57:VAL:HG11	1.94	0.66
2:M:98:ALA:HA	2:M:100:GLU:N	2.10	0.66
1:L:241:VAL:O	1:L:244:SER:CB	2.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:MET:CE	4:L:283:BCL:HMD1	2.25	0.66
2:M:72:ILE:C	2:M:74:PHE:N	2.49	0.66
3:H:34:GLU:OE2	3:H:59:PRO:HB3	1.95	0.66
3:H:170:ASP:OD2	3:H:177:ARG:CZ	2.43	0.66
1:L:69:PRO:HB3	1:L:78:ALA:HB2	1.75	0.66
2:M:85:PHE:O	2:M:89:LEU:HB2	1.95	0.66
3:H:37:ARG:O	3:H:39:GLY:N	2.29	0.66
3:H:64:PHE:N	3:H:73:LEU:O	2.22	0.66
3:H:156:CYS:SG	3:H:209:SER:N	2.68	0.66
1:L:49:ILE:HA	1:L:89:ILE:HD11	1.75	0.66
1:L:182:THR:O	1:L:185:LEU:HD23	1.94	0.66
2:M:46:GLN:HE21	2:M:48:GLY:C	1.98	0.66
2:M:87:ARG:CG	2:M:88:ASP:CG	2.63	0.66
2:M:154:ILE:O	2:M:158:MET:N	2.28	0.66
2:M:159:VAL:O	2:M:162:PHE:N	2.27	0.66
3:H:40:TYR:H	3:H:42:LEU:HD11	1.57	0.66
3:H:155:GLY:O	3:H:206:ASN:HA	1.96	0.66
1:L:60:ASN:CB	1:L:63:LEU:HD12	2.24	0.66
1:L:222:TYR:HD1	1:L:223:SER:N	1.87	0.66
2:M:131:GLY:O	2:M:134:TYR:HB2	1.93	0.66
3:H:184:LYS:HA	3:H:184:LYS:HE3	1.76	0.66
1:L:51:TRP:CH2	1:L:80:LEU:CD1	2.79	0.66
1:L:212:GLU:O	1:L:215:PHE:N	2.27	0.66
1:L:242:PHE:HE1	1:L:243:PHE:HD1	1.44	0.66
1:L:244:SER:OG	4:L:283:BCL:HMA2	1.95	0.66
2:M:82:PRO:O	2:M:83:ALA:C	2.33	0.66
2:M:157:TRP:HB2	4:M:310:BCL:H92	1.77	0.66
2:M:238:ILE:HD11	2:M:263:GLU:N	2.10	0.66
3:H:27:LEU:HD12	3:H:28:ILE:HG13	1.66	0.66
3:H:140:PHE:HZ	3:H:171:ILE:HG23	1.61	0.66
1:L:119:PHE:HE1	1:L:238:LEU:CD1	2.09	0.66
1:L:135:ARG:CB	1:L:136:PRO:HD3	2.15	0.66
2:M:50:ILE:CG2	2:M:51:TYR:N	2.59	0.66
3:H:103:ASP:C	3:H:106:LYS:NZ	2.49	0.66
1:L:53:ALA:O	1:L:59:TRP:HB3	1.95	0.66
1:L:119:PHE:CE1	1:L:238:LEU:CD1	2.78	0.66
2:M:152:SER:CA	2:M:277:THR:HG21	2.24	0.66
1:L:33:PHE:O	1:L:33:PHE:CG	2.39	0.66
1:L:232:LEU:C	1:L:235:LEU:HB2	2.15	0.66
2:M:228:ARG:HH12	3:H:241:LEU:HD11	1.61	0.66
2:M:237:GLN:OE1	2:M:244:ALA:CB	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:275:LEU:HA	2:M:278:LEU:HB3	1.77	0.66
3:H:105:MET:N	3:H:106:LYS:NZ	2.44	0.66
1:L:86:TRP:O	1:L:87:GLN:O	2.14	0.65
2:M:72:ILE:C	2:M:74:PHE:H	1.97	0.65
2:M:228:ARG:NH1	2:M:228:ARG:CG	2.40	0.65
3:H:104:PRO:HG3	3:H:243:TYR:CE2	2.31	0.65
3:H:206:ASN:O	3:H:207:ALA:C	2.35	0.65
1:L:85:LEU:HA	1:L:88:ILE:HD12	1.78	0.65
2:M:109:LEU:CD2	2:M:110:LYS:N	2.47	0.65
2:M:201:PHE:CG	2:M:282:ILE:HG22	2.32	0.65
3:H:124:ASP:O	3:H:125:GLY:C	2.33	0.65
1:L:113:ILE:HG22	1:L:114:GLY:N	2.11	0.65
2:M:275:LEU:CD1	2:M:278:LEU:HD23	2.25	0.65
1:L:47:ILE:CG2	1:L:48:LEU:N	2.59	0.65
1:L:48:LEU:CD1	1:L:89:ILE:CG1	2.73	0.65
1:L:208:THR:CB	1:L:211:HIS:CD2	2.69	0.65
1:L:226:THR:CG2	2:M:232:GLU:HB2	2.25	0.65
2:M:214:LEU:C	2:M:214:LEU:HD12	2.16	0.65
3:H:187:SER:OG	3:H:188:THR:N	2.30	0.65
3:H:235:GLY:O	3:H:238:ALA:N	2.29	0.65
2:M:120:PHE:O	2:M:121:PHE:HD1	1.75	0.65
3:H:30:TYR:O	3:H:31:LEU:C	2.35	0.65
1:L:10:ARG:HH21	3:H:95:GLY:C	2.00	0.65
1:L:175:ILE:HG23	1:L:179:PHE:HE1	1.62	0.65
1:L:248:MET:CE	4:L:283:BCL:C2D	2.69	0.65
2:M:21:THR:HG22	2:M:140:LEU:HD11	1.79	0.65
2:M:204:LEU:CA	2:M:207:ALA:HB3	2.25	0.65
2:M:209:LEU:HD23	2:M:276:VAL:HG11	1.78	0.65
3:H:191:LEU:HD21	3:H:213:PHE:CE1	2.32	0.65
1:L:139:MET:O	1:L:141:ALA:N	2.30	0.65
2:M:128:SER:OG	2:M:129:TRP:N	2.25	0.65
2:M:233:ARG:HH21	3:H:122:GLU:CD	1.98	0.65
3:H:20:PHE:C	3:H:20:PHE:CD1	2.70	0.65
1:L:20:ASN:O	1:L:23:ASP:N	2.30	0.65
1:L:208:THR:HG23	1:L:211:HIS:NE2	2.08	0.65
2:M:236:GLU:OE2	3:H:122:GLU:HA	1.97	0.65
1:L:11:VAL:CG1	3:H:87:LEU:HD21	2.27	0.65
1:L:97:PHE:HE1	4:L:283:BCL:H143	1.54	0.65
2:M:128:SER:C	2:M:130:TRP:N	2.48	0.65
3:H:75:VAL:HB	3:H:76:PRO:HD3	1.77	0.65
1:L:124:ALA:C	1:L:126:LEU:N	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:LEU:HD12	1:L:187:LEU:O	1.97	0.64
2:M:242:GLY:HA2	3:H:115:VAL:CG1	2.18	0.64
3:H:42:LEU:HD21	3:H:76:PRO:HA	1.77	0.64
3:H:115:VAL:CG1	3:H:116:ALA:N	2.58	0.64
3:H:171:ILE:HD12	3:H:171:ILE:N	2.12	0.64
3:H:215:GLY:O	3:H:216:ILE:C	2.36	0.64
1:L:185:LEU:CD2	1:L:185:LEU:N	2.59	0.64
1:L:215:PHE:HZ	2:M:133:THR:HG22	1.60	0.64
1:L:248:MET:C	1:L:250:ILE:H	1.97	0.64
3:H:116:ALA:HA	3:H:228:LEU:HD12	1.76	0.64
1:L:86:TRP:CE3	1:L:87:GLN:CA	2.79	0.64
2:M:88:ASP:O	2:M:92:PHE:CD2	2.50	0.64
3:H:193:MET:O	3:H:195:MET:O	2.16	0.64
3:H:204:HIS:CE1	3:H:205:VAL:HG13	2.33	0.64
1:L:123:PHE:CD1	1:L:238:LEU:HD21	2.32	0.64
1:L:171:PRO:HG3	1:L:263:TRP:CZ2	2.32	0.64
2:M:57:VAL:HG23	2:M:58:LEU:H	1.47	0.64
2:M:152:SER:CB	2:M:277:THR:CG2	2.75	0.64
1:L:16:LEU:CB	1:L:106:GLU:OE2	2.45	0.64
1:L:25:TRP:CZ2	1:L:110:LYS:HE3	2.33	0.64
1:L:94:THR:HG23	1:L:129:LEU:CD1	2.27	0.64
1:L:159:ASN:O	1:L:160:THR:C	2.36	0.64
1:L:171:PRO:C	1:L:173:HIS:N	2.50	0.64
1:L:173:HIS:HA	1:L:247:CYS:SG	2.37	0.64
2:M:119:SER:OG	2:M:120:PHE:N	2.25	0.64
2:M:275:LEU:O	2:M:278:LEU:N	2.30	0.64
3:H:105:MET:N	3:H:106:LYS:HZ1	1.95	0.64
3:H:182:GLU:CA	3:H:187:SER:O	2.45	0.64
1:L:48:LEU:HD13	1:L:85:LEU:HD12	1.79	0.64
2:M:164:ARG:CZ	2:M:168:MET:CE	2.76	0.64
2:M:208:PHE:C	2:M:276:VAL:CG2	2.65	0.64
1:L:67:TYR:N	1:L:67:TYR:HD1	1.95	0.64
2:M:187:ASN:ND2	2:M:187:ASN:C	2.51	0.64
1:L:215:PHE:HE1	1:L:219:LEU:CD2	2.03	0.64
2:M:35:PHE:CD2	2:M:39:LEU:HD23	2.33	0.64
2:M:66:TRP:HZ2	7:M:308:BOG:H1'1	1.62	0.64
2:M:117:ILE:HG22	2:M:118:ALA:N	2.11	0.64
3:H:39:GLY:HA2	3:H:42:LEU:CD2	2.27	0.64
1:L:85:LEU:O	1:L:89:ILE:HB	1.98	0.64
1:L:205:GLU:HA	3:H:65:ILE:HG23	1.75	0.64
1:L:241:VAL:HG21	5:L:284:BPH:HBC3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:44:ASN:N	3:H:44:ASN:HD22	1.96	0.64
1:L:97:PHE:CZ	4:L:283:BCL:C12	2.78	0.64
1:L:175:ILE:O	1:L:178:SER:N	2.31	0.64
2:M:12:VAL:HG13	2:M:13:ARG:N	2.13	0.64
2:M:175:VAL:HG22	2:M:185:TRP:CE2	2.33	0.64
3:H:196:VAL:HG12	3:H:205:VAL:HB	1.79	0.64
1:L:75:LEU:HG	1:L:140:GLY:C	2.18	0.63
2:M:138:GLN:O	2:M:139:ALA:C	2.36	0.63
2:M:298:GLY:O	2:M:301:HIS:N	2.29	0.63
1:L:135:ARG:O	1:L:139:MET:HE2	1.98	0.63
1:L:226:THR:CG2	2:M:232:GLU:CB	2.76	0.63
2:M:150:PHE:CE1	5:M:312:BPH:C4D	2.81	0.63
3:H:31:LEU:O	3:H:32:GLN:O	2.16	0.63
1:L:93:ALA:HB1	1:L:97:PHE:CD2	2.33	0.63
3:H:208:LEU:O	3:H:209:SER:C	2.36	0.63
1:L:123:PHE:CD2	1:L:238:LEU:CD2	2.81	0.63
3:H:168:TRP:NE1	3:H:190:LEU:HD13	2.13	0.63
1:L:67:TYR:N	1:L:67:TYR:CD1	2.66	0.63
1:L:206:MET:CB	3:H:65:ILE:O	2.46	0.63
2:M:34:PRO:HA	2:M:45:ALA:O	1.99	0.63
2:M:197:PHE:HZ	4:M:310:BCL:HBB1	1.52	0.63
2:M:208:PHE:CB	2:M:276:VAL:CG2	2.77	0.63
3:H:175:MET:O	3:H:177:ARG:N	2.30	0.63
1:L:241:VAL:HG12	1:L:242:PHE:H	1.58	0.63
5:L:284:BPH:OBB	5:L:284:BPH:HHC	1.97	0.63
1:L:108:CYS:O	1:L:110:LYS:N	2.32	0.63
1:L:109:ARG:HE	1:L:109:ARG:CA	2.10	0.63
1:L:135:ARG:HG2	1:L:139:MET:CE	2.29	0.63
1:L:226:THR:CG2	2:M:232:GLU:O	2.47	0.63
1:L:244:SER:O	1:L:247:CYS:HB2	1.98	0.63
2:M:114:LEU:HD12	2:M:114:LEU:N	2.06	0.63
3:H:151:LEU:CD2	3:H:203:VAL:CG2	2.73	0.63
2:M:156:LEU:HD23	2:M:156:LEU:C	2.19	0.63
2:M:197:PHE:CE2	4:M:310:BCL:HMC2	2.34	0.63
3:H:12:LEU:HD22	3:H:13:ALA:N	2.14	0.63
3:H:42:LEU:HD23	3:H:76:PRO:HA	1.80	0.63
1:L:48:LEU:CD1	1:L:89:ILE:CD1	2.77	0.63
1:L:109:ARG:HE	1:L:109:ARG:HA	1.63	0.63
1:L:133:LEU:HD13	1:L:137:VAL:HG21	1.76	0.63
1:L:147:PRO:CD	1:L:156:TRP:HB2	2.27	0.63
1:L:193:LEU:CD2	6:L:285:U10:C3	2.73	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:25:ASN:HD22	2:M:26:LEU:N	1.97	0.63
2:M:152:SER:HB3	2:M:277:THR:CG2	2.29	0.63
3:H:203:VAL:O	3:H:204:HIS:HB2	1.99	0.63
2:M:157:TRP:O	2:M:159:VAL:N	2.32	0.62
1:L:54:VAL:HG12	1:L:55:LEU:H	1.64	0.62
1:L:177:ILE:CD1	4:L:283:BCL:C2B	2.76	0.62
1:L:181:PHE:HE1	4:M:310:BCL:HBA2	1.63	0.62
2:M:38:LEU:HD12	2:M:38:LEU:H	1.64	0.62
2:M:164:ARG:CZ	2:M:168:MET:HE1	2.30	0.62
2:M:243:THR:HG21	2:M:247:ARG:HH21	1.64	0.62
1:L:185:LEU:CA	1:L:188:ALA:CB	2.59	0.62
1:L:219:LEU:CA	2:M:132:ARG:NH2	2.60	0.62
2:M:35:PHE:CD1	2:M:39:LEU:HD22	2.34	0.62
2:M:51:TYR:HE1	2:M:53:GLY:HA3	1.64	0.62
3:H:27:LEU:HB2	3:H:32:GLN:OE1	1.99	0.62
1:L:21:LEU:HD12	1:L:22:PHE:CD1	2.33	0.62
1:L:113:ILE:HD12	2:M:226:VAL:CG2	2.27	0.62
2:M:96:PRO:C	2:M:98:ALA:H	2.02	0.62
1:L:152:THR:O	1:L:154:LEU:N	2.32	0.62
1:L:181:PHE:CE1	4:M:310:BCL:H11	2.34	0.62
1:L:188:ALA:HB2	5:M:312:BPH:HBC2	1.81	0.62
1:L:227:LEU:CD2	1:L:231:ARG:HH11	2.13	0.62
2:M:73:TRP:CG	2:M:114:LEU:HD21	2.35	0.62
2:M:76:TYR:O	2:M:76:TYR:HD1	1.83	0.62
3:H:20:PHE:HD1	3:H:21:TRP:N	1.98	0.62
3:H:177:ARG:NH1	3:H:177:ARG:HG3	2.14	0.62
1:L:232:LEU:CG	2:M:42:PHE:CZ	2.77	0.62
2:M:88:ASP:CA	2:M:92:PHE:CE2	2.83	0.62
3:H:132:LYS:HB3	3:H:133:PRO:CD	2.28	0.62
1:L:54:VAL:HG12	1:L:55:LEU:N	2.13	0.62
1:L:113:ILE:HD12	2:M:225:ALA:O	2.00	0.62
1:L:159:ASN:O	1:L:163:THR:N	2.33	0.62
2:M:215:LEU:HA	2:M:218:MET:HB2	1.81	0.62
2:M:242:GLY:O	2:M:243:THR:C	2.37	0.62
3:H:39:GLY:CA	3:H:42:LEU:HD11	2.28	0.62
3:H:56:PHE:CE1	3:H:57:PRO:HD2	2.32	0.62
3:H:183:LEU:HD11	3:H:189:ARG:CD	2.28	0.62
1:L:64:ILE:HD12	1:L:64:ILE:C	2.20	0.62
2:M:103:LEU:CD1	2:M:166:ILE:HA	2.30	0.62
2:M:277:THR:O	2:M:277:THR:CG2	2.48	0.62
1:L:111:LEU:HD21	2:M:251:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:133:LEU:CD1	1:L:137:VAL:HG23	2.25	0.62
1:L:155:ASP:O	1:L:157:VAL:N	2.33	0.62
1:L:206:MET:HB3	3:H:65:ILE:O	1.98	0.62
1:L:222:TYR:O	1:L:223:SER:HB3	1.99	0.62
3:H:27:LEU:CD2	3:H:32:GLN:NE2	2.39	0.62
3:H:44:ASN:ND2	3:H:44:ASN:H	1.97	0.62
1:L:15:THR:HG21	1:L:19:GLY:N	2.15	0.62
1:L:193:LEU:HD23	6:L:285:U10:C2	2.30	0.62
3:H:115:VAL:HG12	3:H:116:ALA:H	1.62	0.62
1:L:10:ARG:NH1	1:L:25:TRP:CD1	2.68	0.61
1:L:79:PRO:C	1:L:81:ALA:H	1.99	0.61
2:M:60:LEU:CD1	5:M:312:BPH:H6C1	2.27	0.61
2:M:193:HIS:ND1	2:M:287:SER:O	2.33	0.61
3:H:27:LEU:C	3:H:32:GLN:OE1	2.39	0.61
1:L:32:GLY:O	1:L:34:PHE:N	2.29	0.61
1:L:208:THR:OG1	1:L:211:HIS:HD2	1.82	0.61
2:M:135:LEU:HA	2:M:138:GLN:HB2	1.83	0.61
2:M:140:LEU:HD12	2:M:140:LEU:N	2.15	0.61
3:H:27:LEU:CB	3:H:32:GLN:OE1	2.47	0.61
3:H:123:LEU:HD23	3:H:126:HIS:O	2.00	0.61
3:H:148:PRO:HA	3:H:151:LEU:HD13	1.81	0.61
1:L:219:LEU:HA	2:M:132:ARG:NH2	2.06	0.61
1:L:248:MET:CE	4:L:283:BCL:CAD	2.78	0.61
4:L:282:BCL:C1	5:M:312:BPH:OBB	2.48	0.61
2:M:37:THR:CG2	2:M:38:LEU:HG	2.30	0.61
2:M:100:GLU:O	2:M:101:TYR:HB2	1.99	0.61
2:M:204:LEU:C	2:M:207:ALA:HB3	2.19	0.61
1:L:78:ALA:HB1	1:L:79:PRO:CD	2.30	0.61
1:L:195:LEU:CB	2:M:145:HIS:CD2	2.72	0.61
2:M:92:PHE:O	2:M:93:SER:HB3	1.99	0.61
3:H:115:VAL:HG13	3:H:116:ALA:H	1.65	0.61
1:L:62:GLN:HB3	1:L:63:LEU:HG	1.81	0.61
1:L:146:PHE:HB2	1:L:156:TRP:CD1	2.35	0.61
1:L:264:GLN:C	1:L:266:TRP:N	2.50	0.61
2:M:230:GLY:O	2:M:232:GLU:N	2.33	0.61
3:H:205:VAL:O	3:H:205:VAL:HG22	2.01	0.61
1:L:222:TYR:HE1	2:M:44:ASN:HB3	1.64	0.61
4:L:283:BCL:C14	5:L:284:BPH:O2A	2.47	0.61
2:M:78:ALA:HB1	2:M:84:VAL:HG12	1.81	0.61
2:M:199:ASN:ND2	2:M:294:TRP:CZ2	2.68	0.61
2:M:284:ILE:CD1	4:M:310:BCL:CED	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:290:VAL:O	2:M:290:VAL:CG1	2.47	0.61
3:H:189:ARG:HH11	3:H:189:ARG:CB	2.07	0.61
1:L:10:ARG:HH21	3:H:95:GLY:CA	2.12	0.61
1:L:206:MET:N	3:H:65:ILE:CG2	2.34	0.61
1:L:255:TRP:CD1	1:L:259:TRP:CZ3	2.88	0.61
2:M:105:PHE:O	2:M:107:ALA:N	2.33	0.61
2:M:186:THR:O	2:M:189:PHE:N	2.34	0.61
3:H:106:LYS:NZ	3:H:106:LYS:H	1.98	0.61
2:M:35:PHE:N	2:M:45:ALA:O	2.23	0.61
2:M:97:PRO:HA	2:M:111:GLU:OE2	2.01	0.61
2:M:102:GLY:C	2:M:104:SER:N	2.48	0.61
2:M:109:LEU:HD23	2:M:114:LEU:CD1	2.21	0.61
2:M:185:TRP:CE3	2:M:186:THR:HA	2.36	0.61
3:H:199:GLN:HE21	3:H:200:SER:N	1.99	0.61
1:L:204:LYS:CB	1:L:207:ARG:HH12	2.09	0.61
4:L:283:BCL:H102	5:L:284:BPH:CHB	2.30	0.61
2:M:70:ILE:HD11	2:M:74:PHE:CE2	2.35	0.61
2:M:120:PHE:CD1	2:M:162:PHE:CE2	2.86	0.61
2:M:206:ILE:HG12	4:M:310:BCL:CHB	2.31	0.61
2:M:238:ILE:HD11	2:M:263:GLU:HA	1.82	0.61
2:M:261:THR:HB	3:H:36:MET:HA	1.82	0.61
1:L:73:TYR:HD2	1:L:82:LYS:HZ1	1.41	0.60
1:L:75:LEU:CD2	1:L:141:ALA:CA	2.79	0.60
1:L:174:MET:HE3	2:M:180:PHE:CZ	2.36	0.60
1:L:175:ILE:HG23	1:L:179:PHE:CE1	2.36	0.60
2:M:37:THR:O	2:M:41:TRP:HD1	1.83	0.60
2:M:264:GLY:O	2:M:267:ARG:N	2.34	0.60
3:H:213:PHE:CD1	3:H:216:ILE:CD1	2.84	0.60
1:L:6:GLU:CD	1:L:10:ARG:HD3	2.20	0.60
4:L:283:BCL:H71	4:L:283:BCL:H41	1.83	0.60
6:L:285:U10:C26	6:L:285:U10:C30	2.79	0.60
2:M:282:ILE:O	2:M:283:GLY:C	2.38	0.60
3:H:20:PHE:C	3:H:22:ILE:H	2.05	0.60
3:H:179:LEU:HD23	3:H:181:VAL:CG2	2.31	0.60
3:H:190:LEU:HD23	3:H:190:LEU:N	2.06	0.60
1:L:133:LEU:HD13	1:L:137:VAL:CG2	2.29	0.60
1:L:215:PHE:CZ	2:M:133:THR:HG22	2.36	0.60
2:M:100:GLU:CA	2:M:172:SER:OG	2.46	0.60
2:M:271:TRP:O	2:M:272:MET:C	2.38	0.60
3:H:123:LEU:HD21	3:H:127:GLY:HA2	1.82	0.60
3:H:132:LYS:O	3:H:168:TRP:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:204:HIS:HB3	3:H:206:ASN:ND2	2.17	0.60
1:L:234:LEU:HD21	1:L:238:LEU:HD12	1.84	0.60
2:M:168:MET:HG3	2:M:173:GLU:HG3	1.82	0.60
2:M:260:ALA:CB	3:H:36:MET:HG3	2.28	0.60
3:H:129:ASN:O	3:H:131:ILE:N	2.34	0.60
3:H:219:ILE:HA	3:H:229:GLU:CG	2.31	0.60
1:L:124:ALA:O	1:L:126:LEU:N	2.34	0.60
1:L:267:VAL:CG1	2:M:87:ARG:CD	2.73	0.60
2:M:13:ARG:NH1	2:M:34:PRO:CB	2.64	0.60
2:M:35:PHE:CD2	2:M:39:LEU:HD21	2.35	0.60
2:M:197:PHE:C	2:M:199:ASN:H	2.03	0.60
3:H:191:LEU:CG	3:H:205:VAL:HG11	2.29	0.60
1:L:154:LEU:O	1:L:158:SER:N	2.34	0.60
1:L:262:TRP:HD1	1:L:263:TRP:CE3	2.18	0.60
6:L:285:U10:H261	6:L:285:U10:C30	2.27	0.60
2:M:13:ARG:CD	3:H:143:SER:OG	2.49	0.60
2:M:114:LEU:O	2:M:118:ALA:N	2.35	0.60
3:H:123:LEU:HD23	3:H:127:GLY:HA2	1.84	0.60
1:L:28:PRO:O	2:M:254:TRP:HA	2.01	0.60
1:L:244:SER:O	1:L:246:LEU:N	2.34	0.60
2:M:222:THR:O	2:M:224:LEU:N	2.34	0.60
2:M:235:LEU:C	2:M:237:GLN:H	2.02	0.60
3:H:94:GLU:N	3:H:94:GLU:OE1	2.34	0.60
1:L:60:ASN:ND2	1:L:63:LEU:CD1	2.64	0.60
1:L:101:ALA:O	1:L:104:GLU:N	2.35	0.60
1:L:107:ILE:HD12	2:M:255:THR:HG1	1.65	0.60
2:M:85:PHE:CD1	2:M:89:LEU:HD12	2.36	0.60
2:M:150:PHE:HE1	5:M:312:BPH:C4D	2.13	0.60
3:H:135:LYS:O	3:H:137:ALA:N	2.35	0.60
3:H:180:GLU:C	3:H:181:VAL:CG2	2.70	0.60
1:L:24:PHE:CD2	1:L:31:VAL:HG21	2.37	0.60
1:L:25:TRP:O	1:L:26:VAL:C	2.40	0.60
1:L:75:LEU:HD21	1:L:141:ALA:CA	2.32	0.60
1:L:123:PHE:CD2	1:L:238:LEU:HD21	2.37	0.60
2:M:17:ASP:C	2:M:18:LEU:CG	2.70	0.60
2:M:129:TRP:HA	2:M:132:ARG:HB2	1.84	0.60
6:M:313:U10:H402	6:M:313:U10:H361	1.83	0.60
3:H:134:MET:N	3:H:166:ASP:OD2	2.35	0.60
3:H:185:ASP:C	3:H:187:SER:N	2.54	0.60
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.84	0.59
1:L:53:ALA:CB	1:L:64:ILE:CB	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:TYR:O	1:L:170:ASN:C	2.40	0.59
2:M:140:LEU:CD1	2:M:140:LEU:H	2.15	0.59
2:M:208:PHE:C	2:M:210:TYR:N	2.54	0.59
2:M:27:ALA:CB	2:M:51:TYR:HA	2.32	0.59
2:M:238:ILE:HG23	3:H:64:PHE:CE2	2.37	0.59
2:M:291:VAL:HG21	2:M:294:TRP:CZ3	2.37	0.59
3:H:60:LYS:O	3:H:60:LYS:CG	2.48	0.59
1:L:144:TYR:HE1	1:L:160:THR:OG1	1.85	0.59
2:M:197:PHE:CE1	4:M:311:BCL:CMD	2.77	0.59
5:M:312:BPH:H4C1	5:M:312:BPH:H8	1.84	0.59
3:H:31:LEU:O	3:H:34:GLU:CB	2.50	0.59
1:L:84:GLY:C	1:L:86:TRP:H	2.04	0.59
1:L:5:PHE:CZ	2:M:246:GLU:HA	2.38	0.59
1:L:113:ILE:HD13	2:M:229:PHE:HE1	1.68	0.59
2:M:164:ARG:HG2	2:M:164:ARG:HH11	1.67	0.59
2:M:35:PHE:HE1	2:M:38:LEU:HD13	1.67	0.59
2:M:37:THR:HG22	2:M:38:LEU:CG	2.31	0.59
2:M:95:GLU:OE1	2:M:176:PRO:HB2	2.03	0.59
2:M:271:TRP:O	2:M:273:ALA:N	2.36	0.59
4:M:310:BCL:HBB3	4:M:310:BCL:CHC	2.32	0.59
3:H:34:GLU:CD	3:H:59:PRO:HB3	2.22	0.59
3:H:134:MET:O	3:H:137:ALA:CB	2.48	0.59
1:L:8:LYS:O	1:L:11:VAL:CG1	2.50	0.59
1:L:73:TYR:CG	1:L:82:LYS:NZ	2.68	0.59
1:L:135:ARG:O	1:L:139:MET:CE	2.51	0.59
2:M:24:VAL:C	2:M:26:LEU:H	2.05	0.59
2:M:205:SER:CA	2:M:279:THR:HG21	2.31	0.59
3:H:103:ASP:O	3:H:106:LYS:CE	2.50	0.59
3:H:204:HIS:HE1	3:H:213:PHE:CZ	2.20	0.59
1:L:171:PRO:O	1:L:174:MET:CB	2.49	0.59
2:M:82:PRO:O	2:M:84:VAL:N	2.36	0.59
2:M:137:ALA:HA	2:M:142:MET:HG3	1.83	0.59
1:L:25:TRP:CZ2	1:L:110:LYS:CE	2.86	0.59
1:L:62:GLN:C	1:L:63:LEU:HG	2.23	0.59
1:L:80:LEU:HD12	1:L:80:LEU:O	2.03	0.59
1:L:90:THR:C	1:L:92:CYS:H	2.05	0.59
2:M:201:PHE:CD2	2:M:282:ILE:HG22	2.38	0.59
3:H:179:LEU:O	3:H:181:VAL:HG23	2.02	0.59
1:L:10:ARG:NH2	1:L:25:TRP:CB	2.63	0.59
1:L:67:TYR:HB3	1:L:68:PRO:HD2	1.85	0.59
1:L:100:TRP:O	1:L:104:GLU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:PHE:HZ	1:L:251:THR:HG21	1.68	0.59
1:L:227:LEU:HD12	2:M:232:GLU:CD	2.23	0.59
1:L:237:SER:O	1:L:238:LEU:C	2.41	0.59
1:L:268:LYS:HD2	1:L:269:LEU:HB2	1.84	0.59
2:M:11:GLN:NE2	3:H:144:ALA:HB3	2.18	0.59
3:H:204:HIS:CD2	3:H:205:VAL:C	2.76	0.59
1:L:92:CYS:O	1:L:96:ALA:CB	2.51	0.58
3:H:183:LEU:N	3:H:187:SER:O	2.36	0.58
1:L:75:LEU:HD23	1:L:142:TRP:N	2.18	0.58
1:L:147:PRO:HD2	1:L:156:TRP:CB	2.32	0.58
1:L:162:TYR:CE1	4:L:283:BCL:HBC3	2.38	0.58
2:M:135:LEU:O	2:M:138:GLN:HB2	2.03	0.58
2:M:193:HIS:O	2:M:293:ASN:HA	2.02	0.58
2:M:249:ALA:HB1	6:M:313:U10:C4M	2.27	0.58
1:L:248:MET:CE	4:L:283:BCL:OBD	2.51	0.58
2:M:36:SER:OG	2:M:37:THR:N	2.36	0.58
2:M:103:LEU:HD13	2:M:166:ILE:HA	1.85	0.58
2:M:224:LEU:C	2:M:226:VAL:H	2.06	0.58
3:H:41:PRO:O	3:H:43:GLU:N	2.37	0.58
3:H:117:ARG:HB2	3:H:227:LEU:HB2	1.85	0.58
1:L:177:ILE:CD1	4:L:283:BCL:CHB	2.81	0.58
2:M:46:GLN:HG2	2:M:47:LEU:N	2.05	0.58
2:M:120:PHE:CE1	2:M:162:PHE:HE2	2.22	0.58
2:M:187:ASN:HD22	2:M:188:ASN:H	0.61	0.58
3:H:191:LEU:HD21	3:H:213:PHE:CZ	2.36	0.58
3:H:238:ALA:C	3:H:240:GLY:N	2.53	0.58
3:H:239:GLY:O	3:H:243:TYR:N	2.26	0.58
1:L:31:VAL:HA	6:M:313:U10:H403	1.83	0.58
2:M:37:THR:HG22	2:M:38:LEU:H	1.69	0.58
2:M:68:PHE:O	2:M:72:ILE:N	2.36	0.58
2:M:71:GLY:O	2:M:74:PHE:HB2	2.04	0.58
2:M:243:THR:O	2:M:244:ALA:C	2.42	0.58
3:H:20:PHE:C	3:H:22:ILE:N	2.56	0.58
1:L:226:THR:HG21	2:M:232:GLU:HB2	1.85	0.58
1:L:269:LEU:HD13	1:L:270:PRO:CD	2.34	0.58
2:M:25:ASN:HD22	2:M:25:ASN:C	2.06	0.58
2:M:114:LEU:O	2:M:117:ILE:N	2.35	0.58
2:M:201:PHE:CE1	2:M:282:ILE:HG21	2.38	0.58
3:H:57:PRO:O	3:H:58:LEU:HB2	2.02	0.58
3:H:116:ALA:CB	3:H:228:LEU:CD1	2.82	0.58
1:L:85:LEU:O	1:L:89:ILE:HD12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:TRP:O	1:L:154:LEU:HD13	2.03	0.58
2:M:35:PHE:CD1	2:M:39:LEU:CD2	2.86	0.58
1:L:101:ALA:O	1:L:104:GLU:CB	2.51	0.58
1:L:127:ALA:CB	4:L:283:BCL:C2	2.81	0.58
1:L:127:ALA:HB3	4:L:283:BCL:H2	1.86	0.58
1:L:146:PHE:HB2	1:L:156:TRP:CG	2.38	0.58
1:L:190:HIS:HA	6:L:285:U10:O2	2.03	0.58
3:H:20:PHE:HE1	3:H:24:LEU:CD1	2.14	0.58
3:H:195:MET:O	3:H:196:VAL:CG2	2.48	0.58
2:M:155:TRP:NE1	2:M:278:LEU:O	2.36	0.58
2:M:204:LEU:C	2:M:207:ALA:CB	2.73	0.58
3:H:39:GLY:N	3:H:42:LEU:HD11	2.18	0.58
3:H:56:PHE:CE1	3:H:57:PRO:CD	2.85	0.58
3:H:96:PHE:C	3:H:97:PRO:O	2.42	0.58
3:H:134:MET:SD	3:H:140:PHE:O	2.61	0.58
3:H:140:PHE:CZ	3:H:171:ILE:HG23	2.38	0.58
3:H:212:LEU:C	3:H:214:ALA:H	2.07	0.58
3:H:213:PHE:HD1	3:H:216:ILE:HD13	1.69	0.58
1:L:15:THR:O	1:L:15:THR:HG22	2.04	0.58
1:L:33:PHE:HD1	1:L:33:PHE:C	1.99	0.58
1:L:262:TRP:CD1	1:L:263:TRP:CE3	2.92	0.58
3:H:116:ALA:CA	3:H:228:LEU:HD12	2.31	0.58
3:H:183:LEU:HD11	3:H:189:ARG:HD2	1.86	0.58
3:H:219:ILE:HG22	3:H:229:GLU:HG2	1.84	0.57
1:L:6:GLU:O	1:L:8:LYS:N	2.37	0.57
4:L:282:BCL:HMD2	4:L:283:BCL:CBB	2.34	0.57
2:M:39:LEU:CD2	2:M:39:LEU:H	2.13	0.57
1:L:78:ALA:HB1	1:L:83:GLY:HA3	1.86	0.57
1:L:98:VAL:CG2	1:L:125:ILE:HD11	2.35	0.57
1:L:179:PHE:CB	1:L:240:ALA:CB	2.58	0.57
2:M:82:PRO:O	2:M:85:PHE:N	2.37	0.57
2:M:205:SER:CB	2:M:279:THR:CG2	2.82	0.57
2:M:281:GLY:O	2:M:285:LEU:HD23	2.04	0.57
2:M:73:TRP:CE2	2:M:114:LEU:CG	2.85	0.57
3:H:123:LEU:O	3:H:130:LYS:HG3	2.03	0.57
3:H:146:LYS:HZ3	3:H:198:VAL:HG12	1.67	0.57
3:H:154:ARG:HA	3:H:160:ILE:HG23	1.86	0.57
3:H:229:GLU:O	3:H:233:ILE:CG1	2.52	0.57
1:L:133:LEU:C	1:L:133:LEU:CD1	2.65	0.57
1:L:216:PHE:C	1:L:218:ASP:H	2.06	0.57
2:M:182:HIS:CE1	2:M:183:LEU:HD12	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:ND2	1:L:63:LEU:HD11	2.19	0.57
2:M:21:THR:CG2	2:M:139:ALA:HB1	2.34	0.57
5:M:312:BPH:C11	5:M:312:BPH:H102	2.18	0.57
3:H:48:THR:CG2	3:H:51:ALA:C	2.73	0.57
1:L:10:ARG:HH21	3:H:95:GLY:HA2	1.61	0.57
1:L:103:ARG:O	1:L:107:ILE:HG12	2.03	0.57
1:L:146:PHE:CE2	4:M:311:BCL:HMC2	2.39	0.57
1:L:174:MET:HE1	2:M:180:PHE:CZ	2.40	0.57
1:L:182:THR:CG2	1:L:236:LEU:HD13	2.34	0.57
1:L:237:SER:C	1:L:239:SER:N	2.58	0.57
1:L:264:GLN:O	1:L:266:TRP:N	2.38	0.57
2:M:58:LEU:O	2:M:61:PHE:N	2.38	0.57
2:M:126:VAL:HG11	2:M:154:ILE:HD12	1.87	0.57
6:M:313:U10:H8	6:M:313:U10:C1M	2.34	0.57
3:H:27:LEU:O	3:H:30:TYR:N	2.37	0.57
3:H:143:SER:O	3:H:144:ALA:CB	2.51	0.57
1:L:84:GLY:O	1:L:85:LEU:C	2.42	0.57
2:M:149:ALA:HB2	2:M:270:ILE:CD1	2.34	0.57
3:H:32:GLN:O	3:H:36:MET:HE1	2.05	0.57
3:H:201:ASN:OD1	3:H:201:ASN:C	2.41	0.57
1:L:69:PRO:CB	1:L:78:ALA:CB	2.81	0.57
1:L:75:LEU:CD2	1:L:141:ALA:C	2.73	0.57
1:L:174:MET:HE1	2:M:180:PHE:CE1	2.39	0.57
2:M:171:TRP:O	2:M:174:ALA:N	2.28	0.57
2:M:260:ALA:CB	3:H:36:MET:CG	2.83	0.57
1:L:155:ASP:O	1:L:158:SER:N	2.38	0.57
2:M:284:ILE:CD1	4:M:310:BCL:HED1	2.35	0.57
3:H:15:LEU:CA	3:H:18:TYR:HD2	2.15	0.57
1:L:98:VAL:O	1:L:102:LEU:HD23	2.05	0.56
1:L:135:ARG:HG2	1:L:139:MET:HE3	1.87	0.56
3:H:17:ILE:CD1	3:H:21:TRP:CD1	2.88	0.56
1:L:121:PHE:HB2	5:L:284:BPH:C2D	2.35	0.56
1:L:263:TRP:CE3	1:L:263:TRP:HA	2.38	0.56
2:M:17:ASP:O	2:M:18:LEU:CG	2.52	0.56
2:M:28:ASN:O	2:M:29:ARG:O	2.22	0.56
2:M:135:LEU:O	2:M:138:GLN:N	2.39	0.56
2:M:204:LEU:C	2:M:207:ALA:H	2.08	0.56
2:M:237:GLN:C	2:M:239:ALA:H	2.07	0.56
3:H:49:PRO:HD2	3:H:50:ALA:O	2.04	0.56
1:L:12:PRO:HD3	3:H:97:PRO:CB	2.35	0.56
1:L:108:CYS:SG	2:M:251:PHE:CE2	2.99	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:114:GLY:N	2:M:225:ALA:HB1	2.20	0.56
1:L:153:HIS:O	1:L:157:VAL:HB	2.06	0.56
1:L:255:TRP:NE1	1:L:259:TRP:CE3	2.73	0.56
2:M:13:ARG:HE	3:H:143:SER:CB	2.18	0.56
2:M:64:LEU:O	2:M:67:PHE:CA	2.54	0.56
2:M:70:ILE:O	2:M:74:PHE:HB2	2.04	0.56
3:H:15:LEU:CA	3:H:18:TYR:CD2	2.76	0.56
3:H:104:PRO:CG	3:H:243:TYR:CE2	2.88	0.56
1:L:111:LEU:HD23	2:M:251:PHE:HB2	1.86	0.56
2:M:132:ARG:C	2:M:134:TYR:N	2.56	0.56
2:M:187:ASN:O	2:M:188:ASN:C	2.43	0.56
2:M:206:ILE:CD1	4:M:310:BCL:C2B	2.83	0.56
3:H:12:LEU:C	3:H:14:SER:N	2.54	0.56
3:H:35:ASN:O	3:H:37:ARG:N	2.39	0.56
3:H:92:VAL:HG13	3:H:93:SER:N	2.20	0.56
1:L:8:LYS:O	1:L:11:VAL:HG13	2.05	0.56
1:L:58:THR:O	1:L:59:TRP:CB	2.50	0.56
1:L:219:LEU:C	2:M:132:ARG:NH2	2.58	0.56
1:L:227:LEU:HD22	1:L:231:ARG:HH11	1.69	0.56
2:M:14:GLY:O	2:M:15:PRO:O	2.24	0.56
2:M:132:ARG:C	2:M:134:TYR:H	2.07	0.56
2:M:205:SER:OG	2:M:279:THR:CG2	2.47	0.56
3:H:96:PHE:O	3:H:97:PRO:O	2.23	0.56
1:L:60:ASN:C	1:L:62:GLN:H	2.08	0.56
1:L:155:ASP:O	1:L:156:TRP:C	2.43	0.56
1:L:182:THR:O	1:L:186:ALA:HB2	2.05	0.56
2:M:26:LEU:CD2	2:M:27:ALA:N	2.67	0.56
2:M:126:VAL:HG11	2:M:154:ILE:CD1	2.35	0.56
2:M:264:GLY:C	2:M:267:ARG:HB2	2.26	0.56
3:H:134:MET:HE3	3:H:141:HIS:HE1	1.70	0.56
3:H:171:ILE:N	3:H:171:ILE:CD1	2.68	0.56
3:H:177:ARG:HH11	3:H:177:ARG:CG	2.17	0.56
1:L:14:GLY:HA3	1:L:110:LYS:HB3	1.88	0.56
1:L:36:VAL:HG22	6:M:313:U10:H412	1.88	0.56
1:L:212:GLU:C	1:L:214:THR:N	2.58	0.56
2:M:21:THR:OG1	2:M:23:ASP:C	2.44	0.56
2:M:110:LYS:HE2	2:M:114:LEU:CD2	2.27	0.56
2:M:271:TRP:CZ3	3:H:31:LEU:CD2	2.87	0.56
3:H:103:ASP:CG	3:H:106:LYS:HZ2	2.04	0.56
3:H:148:PRO:HB2	3:H:164:VAL:HG11	1.88	0.56
3:H:177:ARG:HG3	3:H:177:ARG:HH11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:PHE:HD1	1:L:41:PHE:CD1	2.22	0.56
1:L:147:PRO:HG2	1:L:152:THR:CG2	2.31	0.56
4:L:283:BCL:C15	5:L:284:BPH:H3A	2.23	0.56
2:M:90:PHE:CG	2:M:179:ILE:CD1	2.88	0.56
2:M:18:LEU:CD1	2:M:18:LEU:N	2.64	0.56
2:M:35:PHE:CE1	2:M:38:LEU:HB2	2.41	0.56
2:M:37:THR:CA	2:M:41:TRP:CD1	2.88	0.56
2:M:58:LEU:O	2:M:59:SER:C	2.44	0.56
2:M:140:LEU:CD1	2:M:140:LEU:N	2.68	0.56
3:H:212:LEU:O	3:H:213:PHE:HB2	2.05	0.56
1:L:175:ILE:HD12	1:L:243:PHE:CE2	2.33	0.56
2:M:218:MET:CE	6:M:313:U10:C1M	2.84	0.56
4:M:310:BCL:H42	5:M:312:BPH:CBB	2.37	0.56
3:H:149:ILE:C	3:H:151:LEU:H	2.08	0.56
1:L:173:HIS:CB	1:L:247:CYS:SG	2.92	0.55
2:M:238:ILE:HG23	3:H:64:PHE:CZ	2.40	0.55
2:M:241:ARG:HB2	2:M:241:ARG:CZ	2.36	0.55
2:M:291:VAL:HG11	2:M:294:TRP:CD2	2.40	0.55
1:L:208:THR:N	1:L:211:HIS:CD2	2.73	0.55
4:L:283:BCL:C11	5:L:284:BPH:HBA2	2.35	0.55
2:M:70:ILE:HD11	2:M:74:PHE:CD2	2.41	0.55
1:L:101:ALA:O	1:L:104:GLU:CA	2.54	0.55
1:L:173:HIS:CA	1:L:247:CYS:SG	2.95	0.55
2:M:107:ALA:HB1	2:M:108:PRO:HD2	1.89	0.55
3:H:151:LEU:C	3:H:164:VAL:HG23	2.18	0.55
1:L:244:SER:O	1:L:245:ALA:C	2.45	0.55
4:L:283:BCL:CBB	4:L:283:BCL:HMB1	2.36	0.55
2:M:90:PHE:CD2	2:M:179:ILE:HB	2.42	0.55
3:H:112:ALA:O	3:H:113:SER:C	2.45	0.55
3:H:183:LEU:CG	3:H:189:ARG:HE	2.20	0.55
1:L:53:ALA:HA	1:L:64:ILE:HD13	1.87	0.55
1:L:185:LEU:CG	1:L:186:ALA:N	2.69	0.55
4:L:283:BCL:H42	5:L:284:BPH:CAB	2.33	0.55
2:M:102:GLY:O	2:M:104:SER:HB2	2.07	0.55
3:H:27:LEU:CD1	3:H:32:GLN:CD	2.58	0.55
3:H:119:ASP:OD1	3:H:226:THR:HG21	2.05	0.55
1:L:39:PHE:C	1:L:41:PHE:N	2.53	0.55
1:L:121:PHE:O	1:L:123:PHE:N	2.40	0.55
1:L:216:PHE:HB3	1:L:223:SER:HB2	1.87	0.55
2:M:23:ASP:O	2:M:25:ASN:N	2.40	0.55
2:M:37:THR:CG2	2:M:38:LEU:CD1	2.76	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:114:LEU:HD13	2:M:114:LEU:N	2.15	0.55
2:M:242:GLY:CA	3:H:115:VAL:HG11	2.18	0.55
3:H:103:ASP:O	3:H:106:LYS:NZ	2.39	0.55
3:H:148:PRO:HA	3:H:151:LEU:HD12	1.88	0.55
1:L:47:ILE:O	1:L:48:LEU:C	2.43	0.55
1:L:147:PRO:CG	1:L:152:THR:HG22	2.31	0.55
1:L:175:ILE:CG2	1:L:176:ALA:N	2.66	0.55
1:L:177:ILE:CG2	1:L:181:PHE:HE2	2.12	0.55
1:L:53:ALA:HB2	1:L:64:ILE:CB	2.37	0.55
1:L:189:LEU:HD11	5:M:312:BPH:HED3	1.89	0.55
1:L:260:VAL:O	1:L:260:VAL:CG1	2.53	0.55
3:H:132:LYS:HZ1	3:H:223:THR:HG21	1.66	0.55
3:H:190:LEU:CD2	3:H:190:LEU:N	2.68	0.55
1:L:232:LEU:CA	2:M:42:PHE:CZ	2.83	0.55
2:M:13:ARG:HD2	2:M:45:ALA:HB1	1.87	0.55
2:M:37:THR:O	2:M:41:TRP:CD1	2.59	0.55
1:L:113:ILE:HG23	2:M:225:ALA:HB1	1.88	0.55
1:L:205:GLU:OE1	3:H:68:HIS:HA	2.06	0.55
2:M:93:SER:HA	2:M:177:TYR:O	2.07	0.55
2:M:105:PHE:O	2:M:106:ALA:C	2.45	0.55
2:M:134:TYR:HD1	2:M:134:TYR:C	2.09	0.55
2:M:204:LEU:O	2:M:207:ALA:CA	2.55	0.55
2:M:270:ILE:O	2:M:270:ILE:HG13	2.05	0.55
3:H:205:VAL:O	3:H:205:VAL:CG2	2.55	0.55
3:H:235:GLY:O	3:H:236:TYR:C	2.46	0.55
1:L:144:TYR:HE1	1:L:160:THR:HG1	1.46	0.54
3:H:27:LEU:CG	3:H:32:GLN:HE22	2.17	0.54
3:H:115:VAL:O	3:H:116:ALA:HB2	2.07	0.54
3:H:197:LYS:N	3:H:204:HIS:O	2.40	0.54
2:M:300:ASN:O	2:M:301:HIS:CD2	2.59	0.54
3:H:119:ASP:HA	3:H:226:THR:OG1	2.07	0.54
3:H:234:CYS:C	3:H:237:VAL:HG23	2.27	0.54
1:L:48:LEU:O	1:L:51:TRP:HB3	2.07	0.54
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.89	0.54
1:L:131:LEU:HD13	1:L:146:PHE:CE2	2.42	0.54
2:M:13:ARG:CZ	2:M:34:PRO:HB3	2.37	0.54
2:M:14:GLY:HA3	3:H:140:PHE:CE1	2.42	0.54
2:M:129:TRP:C	2:M:129:TRP:CD1	2.80	0.54
2:M:218:MET:CE	2:M:252:TRP:CD2	2.89	0.54
1:L:25:TRP:HA	1:L:29:PHE:O	2.07	0.54
1:L:48:LEU:CD1	1:L:85:LEU:HD12	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:64:ILE:HD12	1:L:65:SER:H	1.72	0.54
5:L:284:BPH:H162	4:M:311:BCL:HBB3	1.87	0.54
2:M:152:SER:O	2:M:153:ALA:C	2.46	0.54
2:M:295:TYR:O	2:M:298:GLY:N	2.39	0.54
3:H:27:LEU:HD12	3:H:28:ILE:H	0.77	0.54
1:L:174:MET:HE3	2:M:180:PHE:HZ	1.71	0.54
2:M:249:ALA:HB1	6:M:313:U10:H4M3	1.83	0.54
2:M:266:HIS:HA	2:M:269:ALA:HB3	1.89	0.54
3:H:27:LEU:CD1	3:H:27:LEU:C	2.69	0.54
3:H:154:ARG:CD	3:H:160:ILE:HG13	2.37	0.54
3:H:218:THR:HG22	3:H:219:ILE:N	2.22	0.54
1:L:8:LYS:NZ	1:L:9:TYR:CE1	2.73	0.54
1:L:69:PRO:CG	1:L:78:ALA:CB	2.86	0.54
1:L:93:ALA:O	1:L:96:ALA:N	2.41	0.54
1:L:102:LEU:O	1:L:103:ARG:C	2.46	0.54
1:L:255:TRP:CZ2	1:L:262:TRP:CA	2.90	0.54
2:M:12:VAL:C	2:M:13:ARG:CG	2.76	0.54
2:M:127:TRP:CE3	2:M:127:TRP:HA	2.42	0.54
2:M:260:ALA:HB1	3:H:36:MET:SD	2.47	0.54
1:L:234:LEU:CD2	1:L:234:LEU:C	2.76	0.54
3:H:168:TRP:CZ3	3:H:223:THR:C	2.81	0.54
1:L:230:HIS:CG	2:M:223:ILE:HG21	2.42	0.54
2:M:88:ASP:HB3	2:M:91:PHE:HB2	1.89	0.54
2:M:262:MET:C	2:M:265:ILE:HG22	2.28	0.54
3:H:173:GLU:O	3:H:174:GLN:CB	2.55	0.54
1:L:54:VAL:CG1	1:L:55:LEU:N	2.71	0.54
1:L:135:ARG:HG3	1:L:135:ARG:HH11	1.70	0.54
1:L:215:PHE:O	1:L:218:ASP:CB	2.48	0.54
2:M:192:VAL:HG12	2:M:193:HIS:CD2	2.42	0.54
2:M:230:GLY:O	2:M:231:GLY:C	2.46	0.54
2:M:279:THR:HG22	2:M:280:GLY:N	2.22	0.54
3:H:32:GLN:O	3:H:36:MET:CE	2.56	0.54
1:L:181:PHE:CE1	4:M:310:BCL:HBA2	2.43	0.54
2:M:209:LEU:O	2:M:209:LEU:CD1	2.47	0.54
3:H:105:MET:HB3	3:H:106:LYS:HZ3	1.73	0.54
3:H:167:ILE:HA	3:H:178:PHE:O	2.08	0.54
3:H:180:GLU:C	3:H:181:VAL:HG23	2.28	0.54
2:M:116:LEU:O	2:M:120:PHE:HB2	2.07	0.53
2:M:284:ILE:O	2:M:284:ILE:CG2	2.56	0.53
3:H:211:ASP:OD1	3:H:211:ASP:N	2.41	0.53
1:L:10:ARG:HH22	1:L:25:TRP:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:TRP:CD2	1:L:87:GLN:N	2.75	0.53
2:M:122:MET:O	2:M:126:VAL:HG23	2.08	0.53
3:H:15:LEU:O	3:H:16:ALA:O	2.26	0.53
3:H:32:GLN:O	3:H:35:ASN:N	2.36	0.53
3:H:201:ASN:OD1	3:H:202:ARG:HB2	2.07	0.53
1:L:26:VAL:O	1:L:29:PHE:N	2.39	0.53
1:L:31:VAL:HG12	1:L:36:VAL:HG23	1.90	0.53
1:L:121:PHE:C	1:L:123:PHE:N	2.61	0.53
1:L:197:ALA:CB	2:M:235:LEU:HD21	2.38	0.53
2:M:136:ARG:NE	2:M:136:ARG:N	2.57	0.53
2:M:238:ILE:CG2	3:H:64:PHE:CZ	2.91	0.53
3:H:131:ILE:HD11	3:H:225:VAL:HG21	1.90	0.53
1:L:184:ALA:O	1:L:187:LEU:N	2.40	0.53
1:L:249:ILE:HG23	1:L:250:ILE:HD12	1.90	0.53
2:M:196:LEU:O	2:M:199:ASN:HB2	2.07	0.53
2:M:259:ASN:C	2:M:259:ASN:HD22	2.12	0.53
1:L:79:PRO:O	1:L:79:PRO:HG2	2.06	0.53
1:L:130:THR:HA	1:L:134:PHE:HD2	1.72	0.53
2:M:126:VAL:CG1	2:M:154:ILE:HD12	2.38	0.53
2:M:128:SER:O	2:M:130:TRP:N	2.42	0.53
2:M:205:SER:HA	2:M:279:THR:HG21	1.89	0.53
3:H:150:GLY:O	3:H:152:PRO:HD3	2.08	0.53
2:M:150:PHE:HD1	5:M:312:BPH:C2D	2.21	0.53
2:M:237:GLN:HA	2:M:240:ASP:O	2.08	0.53
2:M:261:THR:C	2:M:263:GLU:H	2.11	0.53
1:L:5:PHE:CZ	3:H:40:TYR:HE2	2.20	0.53
1:L:110:LYS:C	1:L:112:GLY:H	2.11	0.53
1:L:244:SER:O	1:L:247:CYS:N	2.41	0.53
4:L:283:BCL:H2C	4:M:310:BCL:CBC	2.35	0.53
2:M:13:ARG:HD2	2:M:45:ALA:CB	2.39	0.53
6:M:313:U10:C8	6:M:313:U10:C1M	2.87	0.53
3:H:191:LEU:CD1	3:H:205:VAL:HG12	2.35	0.53
1:L:186:ALA:C	2:M:216:PHE:CE2	2.74	0.53
1:L:197:ALA:HB1	2:M:235:LEU:HD23	1.90	0.53
2:M:6:ILE:HG22	2:M:7:PHE:HB3	1.91	0.53
2:M:80:TRP:O	2:M:80:TRP:CG	2.61	0.53
2:M:187:ASN:O	2:M:190:SER:HB3	2.08	0.53
3:H:17:ILE:O	3:H:17:ILE:HG23	2.07	0.53
3:H:63:THR:HA	3:H:74:THR:HA	1.91	0.53
3:H:127:GLY:O	3:H:128:HIS:C	2.45	0.53
3:H:219:ILE:HA	3:H:229:GLU:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:228:LEU:HD22	3:H:232:LYS:HD2	1.88	0.53
1:L:233:GLY:C	1:L:235:LEU:N	2.62	0.53
2:M:152:SER:C	2:M:154:ILE:N	2.61	0.53
2:M:206:ILE:HG12	4:M:310:BCL:HHB	1.90	0.53
2:M:289:THR:C	2:M:291:VAL:N	2.53	0.53
3:H:185:ASP:C	3:H:187:SER:H	2.12	0.53
3:H:194:GLN:N	3:H:194:GLN:NE2	2.52	0.53
3:H:199:GLN:NE2	3:H:200:SER:OG	2.41	0.53
3:H:213:PHE:HD1	3:H:216:ILE:CD1	2.22	0.53
1:L:94:THR:HG21	1:L:129:LEU:HD11	1.79	0.53
3:H:19:SER:HA	3:H:22:ILE:HD12	1.91	0.53
3:H:65:ILE:HG22	3:H:65:ILE:O	2.09	0.53
1:L:16:LEU:HB2	1:L:106:GLU:HG2	1.90	0.52
1:L:73:TYR:CD1	1:L:78:ALA:HB2	2.44	0.52
1:L:160:THR:O	1:L:164:TYR:HD1	1.92	0.52
1:L:173:HIS:O	1:L:175:ILE:N	2.42	0.52
2:M:115:TRP:HE3	2:M:116:LEU:N	2.07	0.52
1:L:114:GLY:CA	2:M:225:ALA:HB1	2.39	0.52
1:L:131:LEU:O	1:L:145:ALA:HA	2.09	0.52
1:L:264:GLN:O	1:L:267:VAL:N	2.42	0.52
2:M:15:PRO:HD2	3:H:140:PHE:HE1	1.65	0.52
2:M:257:GLY:O	2:M:258:PHE:CB	2.44	0.52
2:M:268:TRP:CG	6:M:313:U10:H111	2.44	0.52
3:H:247:LYS:O	3:H:248:ARG:HG3	2.08	0.52
1:L:123:PHE:O	1:L:126:LEU:N	2.42	0.52
1:L:130:THR:HA	1:L:134:PHE:CD2	2.45	0.52
1:L:177:ILE:HG23	1:L:181:PHE:CE2	2.43	0.52
2:M:97:PRO:O	2:M:99:PRO:O	2.27	0.52
2:M:238:ILE:HD11	2:M:263:GLU:CB	2.38	0.52
2:M:281:GLY:O	2:M:285:LEU:CD2	2.58	0.52
6:M:313:U10:C4M	6:M:313:U10:O5	2.57	0.52
3:H:63:THR:HG23	3:H:74:THR:CB	2.38	0.52
3:H:115:VAL:HG13	3:H:116:ALA:N	2.22	0.52
1:L:185:LEU:O	1:L:189:LEU:N	2.40	0.52
2:M:65:MET:CE	2:M:121:PHE:CB	2.83	0.52
2:M:81:ASN:O	2:M:82:PRO:O	2.27	0.52
6:M:313:U10:C36	6:M:313:U10:C40	2.88	0.52
3:H:106:LYS:H	3:H:106:LYS:CE	2.23	0.52
3:H:121:PRO:HB3	3:H:225:VAL:O	2.09	0.52
3:H:128:HIS:C	3:H:130:LYS:N	2.63	0.52
3:H:191:LEU:HD11	3:H:205:VAL:HG12	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:196:VAL:CG2	3:H:196:VAL:O	2.57	0.52
1:L:15:THR:HG21	1:L:19:GLY:O	2.10	0.52
1:L:33:PHE:O	1:L:33:PHE:CE1	2.50	0.52
2:M:9:GLN:HE22	3:H:197:LYS:CD	2.21	0.52
2:M:162:PHE:O	2:M:163:ILE:O	2.28	0.52
3:H:108:GLY:CA	3:H:114:TRP:CZ3	2.89	0.52
3:H:191:LEU:CD2	3:H:213:PHE:CZ	2.92	0.52
3:H:212:LEU:O	3:H:213:PHE:CB	2.57	0.52
1:L:15:THR:CG2	1:L:19:GLY:N	2.72	0.52
1:L:216:PHE:C	1:L:218:ASP:N	2.63	0.52
2:M:200:PRO:HG3	2:M:297:TRP:CZ3	2.45	0.52
2:M:261:THR:O	2:M:262:MET:C	2.46	0.52
3:H:142:VAL:O	3:H:142:VAL:CG1	2.57	0.52
1:L:193:LEU:O	1:L:195:LEU:N	2.42	0.52
1:L:255:TRP:HZ2	1:L:262:TRP:CA	2.22	0.52
1:L:255:TRP:CZ2	1:L:262:TRP:HA	2.44	0.52
2:M:139:ALA:CB	2:M:140:LEU:HD12	2.40	0.52
1:L:11:VAL:HA	3:H:98:HIS:O	2.09	0.52
1:L:177:ILE:HG13	4:L:282:BCL:OBD	2.10	0.52
1:L:187:LEU:CD2	2:M:216:PHE:CD2	2.87	0.52
1:L:232:LEU:CD1	2:M:42:PHE:HE2	2.22	0.52
6:M:313:U10:H402	6:M:313:U10:C36	2.40	0.52
3:H:214:ALA:O	3:H:215:GLY:C	2.48	0.52
1:L:97:PHE:HE1	4:L:283:BCL:C13	2.16	0.52
1:L:129:LEU:O	1:L:133:LEU:HB3	2.10	0.52
1:L:133:LEU:O	1:L:137:VAL:N	2.33	0.52
1:L:217:ARG:HA	1:L:221:GLY:HA2	1.92	0.52
4:L:283:BCL:C4	5:L:284:BPH:C3B	2.88	0.52
2:M:261:THR:OG1	3:H:40:TYR:CD1	2.63	0.52
3:H:31:LEU:O	3:H:34:GLU:N	2.43	0.52
3:H:31:LEU:O	3:H:34:GLU:HB2	2.10	0.52
3:H:151:LEU:HB3	3:H:203:VAL:HG23	1.89	0.52
2:M:35:PHE:O	2:M:45:ALA:HA	2.10	0.52
2:M:186:THR:O	2:M:189:PHE:CA	2.57	0.52
1:L:51:TRP:CZ2	1:L:80:LEU:CD1	2.93	0.51
1:L:60:ASN:HD22	1:L:63:LEU:CD1	2.20	0.51
2:M:162:PHE:O	2:M:163:ILE:C	2.47	0.51
4:M:310:BCL:C4	5:M:312:BPH:CBB	2.88	0.51
3:H:94:GLU:C	3:H:96:PHE:N	2.34	0.51
3:H:204:HIS:CD2	3:H:205:VAL:O	2.63	0.51
1:L:53:ALA:HB1	1:L:59:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:ALA:CB	5:M:312:BPH:HBC2	2.41	0.51
1:L:228:GLY:HA2	1:L:231:ARG:HD3	1.92	0.51
2:M:115:TRP:O	2:M:119:SER:HB3	2.11	0.51
2:M:203:GLY:CA	4:M:311:BCL:OBD	2.57	0.51
3:H:178:PHE:CD2	3:H:192:PRO:HA	2.45	0.51
1:L:10:ARG:HH22	3:H:95:GLY:CA	2.15	0.51
1:L:75:LEU:CD2	1:L:141:ALA:HA	2.41	0.51
1:L:75:LEU:CD2	1:L:142:TRP:N	2.73	0.51
1:L:195:LEU:HB3	2:M:145:HIS:NE2	2.25	0.51
2:M:71:GLY:C	2:M:74:PHE:HB2	2.30	0.51
3:H:38:GLU:O	3:H:76:PRO:CA	2.59	0.51
3:H:131:ILE:HG13	3:H:131:ILE:O	2.08	0.51
1:L:46:ILE:HA	1:L:49:ILE:HG22	1.90	0.51
1:L:116:HIS:CE1	2:M:225:ALA:CA	2.89	0.51
1:L:117:ILE:HG21	2:M:252:TRP:CH2	2.45	0.51
1:L:237:SER:C	1:L:239:SER:H	2.14	0.51
2:M:236:GLU:CB	3:H:122:GLU:HG3	2.40	0.51
2:M:295:TYR:O	2:M:296:VAL:O	2.28	0.51
3:H:184:LYS:C	3:H:184:LYS:HD3	2.30	0.51
3:H:226:THR:CG2	3:H:229:GLU:OE1	2.59	0.51
3:H:233:ILE:O	3:H:237:VAL:CG2	2.56	0.51
1:L:181:PHE:HE1	4:M:310:BCL:CBA	2.24	0.51
1:L:249:ILE:CG2	1:L:250:ILE:HD12	2.41	0.51
2:M:24:VAL:O	2:M:24:VAL:HG12	2.10	0.51
2:M:50:ILE:CG2	2:M:52:LEU:HG	2.40	0.51
2:M:209:LEU:H	2:M:276:VAL:HG22	1.70	0.51
3:H:31:LEU:O	3:H:32:GLN:C	2.48	0.51
3:H:85:ILE:C	3:H:87:LEU:N	2.64	0.51
1:L:85:LEU:CA	1:L:88:ILE:HD12	2.41	0.51
1:L:119:PHE:CD1	1:L:120:ALA:N	2.79	0.51
2:M:65:MET:HE1	2:M:121:PHE:HB3	1.91	0.51
2:M:109:LEU:HD13	2:M:110:LYS:H	1.75	0.51
4:M:310:BCL:HBB2	4:M:310:BCL:HHC	1.90	0.51
1:L:113:ILE:HG23	2:M:225:ALA:CB	2.40	0.51
1:L:208:THR:C	1:L:211:HIS:HB2	2.26	0.51
1:L:232:LEU:HG	2:M:42:PHE:HZ	1.69	0.51
1:L:238:LEU:O	1:L:238:LEU:HD23	2.11	0.51
2:M:16:ALA:HB1	2:M:32:VAL:CG2	2.29	0.51
2:M:70:ILE:HD13	2:M:71:GLY:N	2.26	0.51
2:M:134:TYR:C	2:M:134:TYR:CD1	2.84	0.51
2:M:204:LEU:O	2:M:205:SER:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:313:U10:O5	6:M:313:U10:H4M2	2.11	0.51
3:H:116:ALA:HA	3:H:228:LEU:HD11	1.87	0.51
1:L:26:VAL:O	1:L:26:VAL:HG12	2.10	0.51
1:L:69:PRO:HG2	1:L:87:GLN:OE1	2.08	0.51
1:L:75:LEU:HD23	1:L:142:TRP:H	1.75	0.51
1:L:135:ARG:CG	1:L:139:MET:HE3	2.41	0.51
1:L:185:LEU:HB3	5:M:312:BPH:C3C	2.38	0.51
1:L:262:TRP:HD1	1:L:263:TRP:CD2	2.27	0.51
2:M:35:PHE:CG	2:M:39:LEU:HD23	2.44	0.51
2:M:114:LEU:O	2:M:117:ILE:CA	2.58	0.51
2:M:239:ALA:O	3:H:73:LEU:HD12	2.11	0.51
3:H:196:VAL:CA	3:H:204:HIS:O	2.54	0.51
1:L:12:PRO:HD2	3:H:98:HIS:C	2.30	0.51
1:L:187:LEU:HD22	2:M:216:PHE:CD1	2.41	0.51
1:L:234:LEU:HD12	2:M:221:ALA:CB	2.40	0.51
1:L:264:GLN:C	1:L:266:TRP:H	2.14	0.51
2:M:12:VAL:CG1	2:M:13:ARG:N	2.74	0.51
2:M:193:HIS:CD2	2:M:193:HIS:N	2.79	0.51
2:M:236:GLU:HG2	3:H:122:GLU:HG3	1.91	0.51
3:H:111:PRO:CB	3:H:242:MET:HB2	2.40	0.51
2:M:13:ARG:NE	3:H:143:SER:OG	2.44	0.51
2:M:264:GLY:O	2:M:267:ARG:CB	2.58	0.51
3:H:239:GLY:O	3:H:240:GLY:C	2.48	0.51
1:L:212:GLU:O	1:L:213:ASP:C	2.49	0.50
2:M:23:ASP:OD1	2:M:24:VAL:HG23	2.11	0.50
2:M:241:ARG:HB3	2:M:241:ARG:NH1	2.09	0.50
2:M:268:TRP:CE2	6:M:313:U10:H111	2.46	0.50
1:L:189:LEU:HD21	5:M:312:BPH:CAD	2.41	0.50
4:L:282:BCL:HMD2	4:L:283:BCL:CAB	2.41	0.50
3:H:27:LEU:CD1	3:H:32:GLN:HE22	2.20	0.50
3:H:132:LYS:CB	3:H:133:PRO:CD	2.89	0.50
1:L:6:GLU:HA	1:L:9:TYR:HD1	1.75	0.50
1:L:11:VAL:HG12	3:H:87:LEU:CD1	2.32	0.50
1:L:11:VAL:O	1:L:12:PRO:O	2.29	0.50
1:L:94:THR:O	1:L:94:THR:HG22	2.11	0.50
1:L:135:ARG:N	1:L:136:PRO:CD	2.74	0.50
1:L:255:TRP:CD1	1:L:259:TRP:CD2	2.99	0.50
2:M:133:THR:HG21	2:M:146:THR:CG2	2.41	0.50
3:H:35:ASN:O	3:H:36:MET:C	2.48	0.50
3:H:183:LEU:HD21	3:H:189:ARG:CD	2.41	0.50
1:L:86:TRP:HE3	1:L:87:GLN:CA	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:128:TYR:HB3	4:L:283:BCL:H61	1.92	0.50
2:M:208:PHE:HB3	2:M:276:VAL:CG2	2.31	0.50
2:M:214:LEU:HG	2:M:215:LEU:N	2.25	0.50
3:H:40:TYR:O	3:H:41:PRO:C	2.49	0.50
3:H:215:GLY:O	3:H:217:PRO:N	2.43	0.50
1:L:46:ILE:O	1:L:49:ILE:HG22	2.11	0.50
1:L:146:PHE:HB3	1:L:156:TRP:CE2	2.47	0.50
1:L:160:THR:O	1:L:161:GLY:O	2.29	0.50
1:L:205:GLU:O	1:L:207:ARG:HD3	2.12	0.50
4:M:310:BCL:H172	5:M:312:BPH:HMB1	1.93	0.50
1:L:40:PHE:HD1	1:L:41:PHE:HD1	1.59	0.50
2:M:155:TRP:CD1	2:M:278:LEU:O	2.65	0.50
2:M:236:GLU:CD	3:H:122:GLU:HG3	2.32	0.50
3:H:154:ARG:HD2	3:H:160:ILE:HG23	1.94	0.50
1:L:5:PHE:O	1:L:7:ARG:N	2.45	0.50
1:L:160:THR:HA	1:L:163:THR:OG1	2.11	0.50
4:L:283:BCL:HMB1	4:L:283:BCL:HBB3	1.94	0.50
2:M:78:ALA:HB1	2:M:84:VAL:CG1	2.41	0.50
2:M:164:ARG:CZ	2:M:168:MET:HE2	2.41	0.50
2:M:290:VAL:O	2:M:291:VAL:CG2	2.52	0.50
3:H:153:VAL:O	3:H:160:ILE:HG22	2.12	0.50
3:H:179:LEU:CD2	3:H:181:VAL:HG22	2.42	0.50
3:H:245:ALA:O	3:H:246:PRO:O	2.30	0.50
1:L:48:LEU:CD1	1:L:89:ILE:HD12	2.39	0.50
1:L:87:GLN:NE2	1:L:142:TRP:HE1	2.10	0.50
1:L:261:ASP:O	1:L:262:TRP:C	2.49	0.50
1:L:262:TRP:HA	1:L:262:TRP:CE3	2.46	0.50
2:M:13:ARG:NE	3:H:143:SER:CB	2.75	0.50
2:M:52:LEU:O	2:M:53:GLY:O	2.30	0.50
2:M:87:ARG:HG3	2:M:88:ASP:CB	2.41	0.50
2:M:213:ALA:O	2:M:217:ALA:HB2	2.12	0.50
3:H:112:ALA:O	3:H:235:GLY:HA3	2.12	0.50
3:H:193:MET:C	3:H:195:MET:H	2.15	0.50
3:H:199:GLN:NE2	3:H:200:SER:N	2.59	0.50
3:H:204:HIS:HD2	3:H:206:ASN:HA	1.76	0.50
1:L:119:PHE:CD1	1:L:119:PHE:C	2.85	0.49
2:M:154:ILE:O	2:M:157:TRP:HB3	2.12	0.49
2:M:196:LEU:HD12	2:M:294:TRP:CD1	2.41	0.49
2:M:196:LEU:O	2:M:196:LEU:HG	2.12	0.49
7:M:308:BOG:O2	7:M:308:BOG:H1'2	2.12	0.49
3:H:233:ILE:HD13	3:H:233:ILE:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:LYS:HB3	3:H:85:ILE:CG2	2.42	0.49
1:L:12:PRO:HG2	3:H:99:ALA:HA	1.93	0.49
2:M:28:ASN:O	2:M:29:ARG:C	2.51	0.49
2:M:35:PHE:CD1	2:M:38:LEU:HD13	2.47	0.49
2:M:204:LEU:O	2:M:206:ILE:N	2.45	0.49
3:H:82:ASP:O	3:H:84:PRO:HD3	2.11	0.49
3:H:207:ALA:C	3:H:247:LYS:NZ	2.62	0.49
1:L:54:VAL:C	1:L:56:GLN:N	2.64	0.49
1:L:108:CYS:SG	2:M:251:PHE:HE2	2.36	0.49
1:L:121:PHE:C	1:L:123:PHE:H	2.14	0.49
1:L:134:PHE:O	1:L:135:ARG:C	2.50	0.49
2:M:89:LEU:CA	2:M:92:PHE:CD2	2.91	0.49
2:M:261:THR:O	2:M:264:GLY:N	2.44	0.49
3:H:40:TYR:O	3:H:42:LEU:HD12	2.01	0.49
3:H:111:PRO:CD	3:H:243:TYR:CE1	2.78	0.49
3:H:210:SER:C	3:H:212:LEU:N	2.43	0.49
1:L:25:TRP:HZ2	2:M:254:TRP:CH2	2.31	0.49
1:L:49:ILE:HA	1:L:89:ILE:CD1	2.42	0.49
1:L:79:PRO:O	1:L:79:PRO:CG	2.61	0.49
2:M:50:ILE:HG23	2:M:52:LEU:HG	1.95	0.49
2:M:208:PHE:CE2	2:M:275:LEU:HB3	2.47	0.49
2:M:230:GLY:C	2:M:232:GLU:N	2.66	0.49
3:H:198:VAL:O	3:H:198:VAL:CG1	2.58	0.49
1:L:46:ILE:CA	1:L:49:ILE:HG22	2.43	0.49
1:L:97:PHE:CE1	4:L:283:BCL:H122	2.38	0.49
1:L:173:HIS:HE1	1:L:177:ILE:HD11	1.72	0.49
1:L:174:MET:CE	2:M:180:PHE:CE1	2.96	0.49
1:L:234:LEU:CD1	2:M:221:ALA:HB2	2.42	0.49
2:M:25:ASN:C	2:M:27:ALA:N	2.63	0.49
2:M:107:ALA:HB1	2:M:112:GLY:HA3	1.95	0.49
2:M:129:TRP:CD1	2:M:129:TRP:O	2.66	0.49
2:M:164:ARG:HH21	2:M:168:MET:HE1	1.73	0.49
3:H:219:ILE:CG2	3:H:225:VAL:HG12	2.43	0.49
3:H:227:LEU:O	3:H:229:GLU:N	2.46	0.49
1:L:10:ARG:NH2	3:H:95:GLY:C	2.64	0.49
1:L:36:VAL:O	1:L:39:PHE:HB3	2.13	0.49
1:L:113:ILE:CD1	2:M:229:PHE:HE1	2.26	0.49
1:L:123:PHE:O	1:L:126:LEU:CA	2.60	0.49
1:L:167:PHE:CD2	4:L:283:BCL:C1D	2.96	0.49
1:L:225:GLY:HA2	6:L:285:U10:H4M1	1.94	0.49
1:L:241:VAL:HG21	5:L:284:BPH:H2C	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:64:LEU:HD12	5:M:312:BPH:C7	2.24	0.49
2:M:191:LEU:HD13	2:M:191:LEU:H	1.76	0.49
2:M:206:ILE:HD11	4:M:310:BCL:NB	2.25	0.49
3:H:27:LEU:O	3:H:28:ILE:C	2.51	0.49
3:H:146:LYS:HZ2	3:H:198:VAL:HG12	1.75	0.49
1:L:48:LEU:HB2	1:L:85:LEU:HD12	1.94	0.49
1:L:98:VAL:HG23	1:L:125:ILE:HD11	1.95	0.49
1:L:149:GLY:O	1:L:150:ILE:C	2.47	0.49
2:M:125:ALA:O	2:M:126:VAL:C	2.50	0.49
2:M:206:ILE:HG12	4:M:310:BCL:HMB3	1.95	0.49
3:H:48:THR:HG23	3:H:51:ALA:C	2.33	0.49
3:H:124:ASP:C	3:H:126:HIS:N	2.64	0.49
1:L:181:PHE:HE1	4:M:310:BCL:CGA	2.25	0.49
2:M:256:MET:O	2:M:257:GLY:O	2.30	0.49
3:H:87:LEU:HD13	3:H:109:VAL:CG1	2.43	0.49
3:H:204:HIS:CD2	3:H:206:ASN:HA	2.48	0.49
1:L:66:VAL:O	1:L:147:PRO:HA	2.13	0.49
1:L:158:SER:O	1:L:162:TYR:HD1	1.96	0.49
1:L:261:ASP:O	1:L:262:TRP:O	2.30	0.49
5:L:284:BPH:HMC3	2:M:213:ALA:HB1	1.95	0.49
2:M:102:GLY:O	2:M:104:SER:CA	2.59	0.49
2:M:108:PRO:HG2	2:M:111:GLU:CB	2.31	0.49
2:M:114:LEU:C	2:M:117:ILE:HB	2.30	0.49
2:M:228:ARG:HH12	3:H:241:LEU:CD1	2.24	0.49
1:L:46:ILE:HA	1:L:49:ILE:HG21	1.92	0.49
1:L:151:TRP:CZ3	2:M:198:TYR:CD1	2.95	0.49
2:M:243:THR:HG22	2:M:247:ARG:CD	2.42	0.49
3:H:189:ARG:CB	3:H:216:ILE:CG2	2.85	0.49
1:L:187:LEU:HA	2:M:216:PHE:CE2	2.48	0.48
4:L:283:BCL:H162	5:L:284:BPH:HBA1	1.95	0.48
2:M:128:SER:C	2:M:130:TRP:H	2.15	0.48
3:H:135:LYS:C	3:H:137:ALA:N	2.64	0.48
1:L:15:THR:HG21	1:L:19:GLY:HA2	1.93	0.48
1:L:20:ASN:C	1:L:22:PHE:N	2.43	0.48
1:L:46:ILE:C	1:L:49:ILE:HG22	2.34	0.48
1:L:135:ARG:NH1	1:L:139:MET:CE	2.76	0.48
2:M:89:LEU:HA	2:M:92:PHE:CE2	2.47	0.48
2:M:120:PHE:HD1	2:M:162:PHE:CE2	2.30	0.48
2:M:296:VAL:C	2:M:298:GLY:N	2.67	0.48
3:H:196:VAL:H	3:H:205:VAL:HA	1.77	0.48
1:L:144:TYR:CE1	1:L:160:THR:OG1	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ASN:OD1	1:L:237:SER:HB3	2.13	0.48
1:L:231:ARG:NH1	2:M:7:PHE:HA	2.29	0.48
1:L:269:LEU:HD22	1:L:270:PRO:N	2.20	0.48
2:M:46:GLN:CG	2:M:48:GLY:O	2.58	0.48
3:H:52:ASN:O	3:H:53:GLN:CB	2.59	0.48
3:H:56:PHE:CD1	3:H:57:PRO:CA	2.92	0.48
1:L:34:PHE:HB3	1:L:99:SER:O	2.13	0.48
1:L:73:TYR:CE1	1:L:78:ALA:HA	2.48	0.48
1:L:147:PRO:CD	1:L:156:TRP:CB	2.91	0.48
1:L:212:GLU:C	1:L:214:THR:H	2.16	0.48
4:L:282:BCL:HMD2	4:L:283:BCL:HBB3	1.96	0.48
2:M:98:ALA:CA	2:M:99:PRO:C	2.80	0.48
2:M:205:SER:CA	2:M:279:THR:CG2	2.91	0.48
3:H:41:PRO:C	3:H:43:GLU:N	2.66	0.48
3:H:170:ASP:O	3:H:174:GLN:HA	2.13	0.48
1:L:182:THR:O	1:L:185:LEU:HD22	2.03	0.48
5:L:284:BPH:HBC3	5:L:284:BPH:H2C	1.34	0.48
2:M:88:ASP:HB2	2:M:92:PHE:HZ	1.64	0.48
2:M:119:SER:HB2	2:M:177:TYR:CZ	2.48	0.48
2:M:154:ILE:HD12	2:M:157:TRP:CE3	2.49	0.48
2:M:222:THR:O	2:M:223:ILE:C	2.51	0.48
3:H:80:SER:O	3:H:81:GLU:CG	2.61	0.48
3:H:157:ASP:OD2	3:H:211:ASP:CG	2.51	0.48
1:L:119:PHE:HD1	1:L:120:ALA:N	2.12	0.48
1:L:147:PRO:HD3	1:L:156:TRP:CD1	2.49	0.48
1:L:167:PHE:HE2	4:L:283:BCL:C2D	2.26	0.48
1:L:265:TRP:CH2	1:L:266:TRP:HE3	2.31	0.48
2:M:72:ILE:CD1	2:M:72:ILE:O	2.62	0.48
2:M:97:PRO:HB3	2:M:112:GLY:HA2	1.94	0.48
2:M:123:PHE:CE1	2:M:127:TRP:CD1	3.02	0.48
2:M:152:SER:C	2:M:154:ILE:H	2.16	0.48
2:M:158:MET:O	2:M:162:PHE:HB2	2.14	0.48
2:M:206:ILE:HA	4:M:310:BCL:HMA1	1.95	0.48
4:M:311:BCL:HBB2	4:M:311:BCL:CMB	2.42	0.48
3:H:135:LYS:O	3:H:136:ALA:C	2.51	0.48
1:L:15:THR:O	1:L:15:THR:CG2	2.61	0.48
1:L:177:ILE:HG21	1:L:181:PHE:CE2	2.41	0.48
1:L:242:PHE:CE1	1:L:243:PHE:HD1	2.29	0.48
3:H:30:TYR:O	3:H:31:LEU:O	2.30	0.48
3:H:82:ASP:O	3:H:82:ASP:CG	2.52	0.48
1:L:65:SER:C	1:L:66:VAL:CG2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:TYR:CE1	1:L:78:ALA:HB2	2.49	0.48
1:L:113:ILE:HD11	2:M:226:VAL:CG2	2.27	0.48
1:L:147:PRO:HD2	1:L:156:TRP:CG	2.48	0.48
1:L:153:HIS:HD2	1:L:154:LEU:H	1.60	0.48
1:L:265:TRP:C	1:L:265:TRP:CE3	2.87	0.48
2:M:78:ALA:CB	2:M:84:VAL:HG12	2.44	0.48
2:M:206:ILE:CG1	4:M:310:BCL:C1B	2.92	0.48
2:M:295:TYR:HB3	2:M:296:VAL:H	1.24	0.48
3:H:208:LEU:C	3:H:208:LEU:HD12	2.30	0.48
3:H:219:ILE:HG22	3:H:229:GLU:CG	2.43	0.48
1:L:15:THR:CG2	1:L:19:GLY:H	2.26	0.48
1:L:116:HIS:NE2	2:M:224:LEU:HB3	2.28	0.48
4:L:282:BCL:HED1	2:M:179:ILE:CG2	2.43	0.48
2:M:38:LEU:C	2:M:40:GLY:N	2.65	0.48
2:M:62:SER:C	2:M:64:LEU:H	2.16	0.48
2:M:121:PHE:C	2:M:123:PHE:H	2.17	0.48
2:M:201:PHE:CD2	2:M:282:ILE:CG2	2.97	0.48
4:M:310:BCL:H3A	4:M:310:BCL:HBA1	1.56	0.48
3:H:153:VAL:HG21	3:H:181:VAL:CG1	2.44	0.48
1:L:25:TRP:CZ2	1:L:110:LYS:NZ	2.79	0.48
1:L:224:ILE:HA	2:M:44:ASN:HB2	1.96	0.48
1:L:225:GLY:CA	3:H:173:GLU:OE2	2.60	0.48
2:M:89:LEU:CA	2:M:92:PHE:CE2	2.97	0.48
2:M:94:LEU:CD2	2:M:114:LEU:HB3	2.31	0.48
3:H:36:MET:HE2	3:H:36:MET:CA	2.27	0.48
3:H:110:GLY:HA3	3:H:243:TYR:OH	2.13	0.48
3:H:120:LEU:CD2	3:H:121:PRO:O	2.59	0.48
3:H:210:SER:HA	3:H:213:PHE:CD2	2.44	0.48
1:L:169:TYR:O	1:L:171:PRO:N	2.47	0.47
1:L:208:THR:H	1:L:211:HIS:CB	2.26	0.47
1:L:255:TRP:CG	1:L:259:TRP:CZ3	3.02	0.47
2:M:116:LEU:O	2:M:120:PHE:CB	2.62	0.47
3:H:56:PHE:CG	3:H:57:PRO:HD2	2.37	0.47
3:H:210:SER:O	3:H:212:LEU:C	2.53	0.47
3:H:240:GLY:O	3:H:241:LEU:O	2.31	0.47
1:L:151:TRP:CE3	1:L:154:LEU:CD2	2.93	0.47
4:L:283:BCL:H102	5:L:284:BPH:C1B	2.43	0.47
2:M:51:TYR:CE1	2:M:53:GLY:HA3	2.47	0.47
2:M:208:PHE:HB2	2:M:276:VAL:HG22	1.97	0.47
3:H:38:GLU:O	3:H:76:PRO:HA	2.14	0.47
1:L:35:GLY:CA	6:M:313:U10:H402	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.44	0.47
1:L:146:PHE:CE2	4:M:311:BCL:CMC	2.97	0.47
1:L:232:LEU:CB	2:M:42:PHE:CZ	2.97	0.47
2:M:67:PHE:CD1	2:M:67:PHE:O	2.67	0.47
2:M:132:ARG:O	2:M:133:THR:C	2.52	0.47
2:M:203:GLY:O	2:M:206:ILE:N	2.47	0.47
3:H:199:GLN:HE21	3:H:200:SER:H	1.62	0.47
1:L:113:ILE:CD1	2:M:226:VAL:HG23	2.37	0.47
1:L:132:VAL:C	1:L:136:PRO:HG2	2.34	0.47
4:L:283:BCL:H42	5:L:284:BPH:OBB	2.13	0.47
2:M:24:VAL:C	2:M:26:LEU:N	2.56	0.47
2:M:66:TRP:CD1	2:M:66:TRP:C	2.86	0.47
2:M:88:ASP:OD1	2:M:91:PHE:HD2	1.97	0.47
2:M:157:TRP:CB	4:M:310:BCL:H92	2.44	0.47
2:M:245:ALA:O	2:M:248:ALA:N	2.43	0.47
3:H:69:GLY:O	3:H:70:ARG:HB2	2.14	0.47
1:L:93:ALA:C	1:L:95:GLY:N	2.62	0.47
4:L:283:BCL:H72	4:M:311:BCL:CAB	2.44	0.47
2:M:53:GLY:O	2:M:57:VAL:HG12	2.14	0.47
2:M:167:LEU:HA	2:M:167:LEU:HD23	1.54	0.47
1:L:17:VAL:CG1	1:L:18:GLY:N	2.51	0.47
1:L:25:TRP:HB2	3:H:95:GLY:O	2.15	0.47
1:L:216:PHE:CE1	1:L:219:LEU:HD23	2.50	0.47
1:L:241:VAL:O	1:L:244:SER:N	2.47	0.47
2:M:21:THR:HG22	2:M:139:ALA:HB1	1.95	0.47
2:M:39:LEU:N	2:M:39:LEU:HD22	2.27	0.47
2:M:121:PHE:C	2:M:123:PHE:N	2.67	0.47
2:M:208:PHE:CD2	2:M:275:LEU:HB3	2.50	0.47
2:M:214:LEU:CG	2:M:215:LEU:N	2.74	0.47
3:H:22:ILE:C	3:H:24:LEU:H	2.17	0.47
3:H:38:GLU:HG3	3:H:76:PRO:HD3	1.96	0.47
3:H:123:LEU:CD2	3:H:126:HIS:O	2.62	0.47
1:L:78:ALA:CB	1:L:79:PRO:HD3	2.45	0.47
1:L:152:THR:O	1:L:153:HIS:C	2.53	0.47
1:L:177:ILE:HD12	4:L:283:BCL:CMB	2.44	0.47
1:L:239:SER:O	1:L:242:PHE:N	2.48	0.47
4:L:282:BCL:HBB2	4:L:282:BCL:CHC	2.38	0.47
2:M:13:ARG:HD3	3:H:143:SER:OG	2.15	0.47
2:M:70:ILE:HG12	2:M:74:PHE:HD2	1.79	0.47
2:M:97:PRO:CB	2:M:111:GLU:OE2	2.62	0.47
2:M:192:VAL:O	2:M:192:VAL:CG1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:196:LEU:O	2:M:199:ASN:CB	2.63	0.47
2:M:242:GLY:O	2:M:243:THR:O	2.33	0.47
4:M:310:BCL:H42	5:M:312:BPH:HBB1	1.96	0.47
3:H:19:SER:O	3:H:20:PHE:O	2.32	0.47
3:H:24:LEU:CD2	3:H:28:ILE:CD1	2.69	0.47
3:H:34:GLU:HB3	3:H:35:ASN:HD22	1.79	0.47
3:H:36:MET:N	3:H:36:MET:HE3	1.98	0.47
3:H:153:VAL:HG23	3:H:164:VAL:HG22	1.97	0.47
3:H:213:PHE:CD1	3:H:216:ILE:HD13	2.49	0.47
3:H:241:LEU:O	3:H:242:MET:C	2.52	0.47
1:L:21:LEU:CD1	1:L:22:PHE:CE1	2.76	0.47
1:L:110:LYS:HG3	1:L:111:LEU:N	2.29	0.47
2:M:88:ASP:C	2:M:92:PHE:CZ	2.79	0.47
2:M:130:TRP:CZ3	2:M:151:LEU:HG	2.50	0.47
2:M:170:SER:HG	2:M:172:SER:HB3	1.78	0.47
2:M:206:ILE:CD1	4:M:311:BCL:HMD1	2.38	0.47
2:M:264:GLY:O	2:M:267:ARG:CA	2.63	0.47
5:M:312:BPH:C11	5:M:312:BPH:H101	2.18	0.47
3:H:36:MET:H	3:H:36:MET:HE2	0.99	0.47
3:H:147:ASN:OD1	3:H:148:PRO:HD2	2.15	0.47
3:H:153:VAL:O	3:H:160:ILE:CG2	2.62	0.47
3:H:191:LEU:HD22	3:H:205:VAL:HG11	1.96	0.47
1:L:78:ALA:CB	1:L:79:PRO:CD	2.93	0.47
2:M:139:ALA:CB	2:M:140:LEU:CD1	2.92	0.47
2:M:168:MET:HG3	2:M:173:GLU:CG	2.45	0.47
2:M:189:PHE:CD1	2:M:189:PHE:O	2.68	0.47
2:M:196:LEU:HD11	2:M:199:ASN:HD22	1.75	0.47
2:M:245:ALA:O	2:M:246:GLU:C	2.54	0.47
3:H:156:CYS:O	3:H:157:ASP:O	2.32	0.47
1:L:98:VAL:HG22	1:L:125:ILE:HD11	1.97	0.47
1:L:133:LEU:C	1:L:136:PRO:HD2	2.35	0.47
1:L:170:ASN:O	1:L:173:HIS:CB	2.57	0.47
1:L:202:LYS:O	1:L:202:LYS:CG	2.63	0.47
4:L:282:BCL:HBA2	4:L:282:BCL:H3A	1.46	0.47
4:L:283:BCL:H2C	4:L:283:BCL:HBC2	1.68	0.47
4:L:283:BCL:H41	5:L:284:BPH:C3B	2.45	0.47
2:M:95:GLU:OE1	2:M:176:PRO:CB	2.62	0.47
2:M:139:ALA:HB3	2:M:140:LEU:HD12	1.94	0.47
2:M:206:ILE:HG13	4:M:310:BCL:CHB	2.43	0.47
2:M:300:ASN:C	2:M:301:HIS:CD2	2.88	0.47
3:H:14:SER:C	3:H:18:TYR:HD2	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:VAL:O	1:L:106:GLU:C	2.53	0.46
1:L:182:THR:C	1:L:184:ALA:N	2.50	0.46
1:L:228:GLY:O	1:L:232:LEU:HB2	2.15	0.46
4:L:282:BCL:HAC1	4:M:310:BCL:C3D	2.45	0.46
2:M:13:ARG:HH11	2:M:13:ARG:HB2	1.80	0.46
2:M:46:GLN:NE2	2:M:49:PRO:HD3	2.26	0.46
2:M:222:THR:HG22	2:M:223:ILE:N	2.30	0.46
3:H:14:SER:O	3:H:18:TYR:CG	2.68	0.46
1:L:49:ILE:N	1:L:89:ILE:HD11	2.30	0.46
1:L:110:LYS:HE2	2:M:254:TRP:CZ3	2.49	0.46
1:L:217:ARG:O	2:M:50:ILE:HA	2.15	0.46
1:L:266:TRP:HD1	1:L:267:VAL:HG22	1.81	0.46
2:M:24:VAL:O	2:M:25:ASN:C	2.49	0.46
2:M:182:HIS:ND1	2:M:183:LEU:HD12	2.30	0.46
2:M:212:SER:C	2:M:214:LEU:N	2.68	0.46
3:H:118:ARG:HH11	3:H:227:LEU:CD1	2.28	0.46
3:H:161:ALA:CB	3:H:210:SER:CB	2.80	0.46
2:M:35:PHE:HE1	2:M:38:LEU:HD22	1.80	0.46
2:M:111:GLU:O	2:M:112:GLY:O	2.33	0.46
2:M:185:TRP:C	2:M:185:TRP:HE3	2.15	0.46
2:M:295:TYR:O	2:M:296:VAL:C	2.53	0.46
3:H:100:PRO:HB3	3:H:109:VAL:CG1	2.45	0.46
6:L:285:U10:C32	2:M:60:LEU:HD21	2.45	0.46
2:M:50:ILE:HG23	2:M:51:TYR:H	1.78	0.46
2:M:131:GLY:O	2:M:132:ARG:C	2.54	0.46
2:M:157:TRP:CE3	2:M:158:MET:HG2	2.51	0.46
2:M:238:ILE:HG12	2:M:263:GLU:HG3	1.96	0.46
3:H:219:ILE:HG22	3:H:229:GLU:CD	2.36	0.46
1:L:264:GLN:O	1:L:265:TRP:C	2.53	0.46
4:L:282:BCL:HED1	2:M:179:ILE:HG22	1.96	0.46
2:M:197:PHE:C	2:M:199:ASN:N	2.68	0.46
2:M:230:GLY:HA2	2:M:232:GLU:OE2	2.16	0.46
3:H:83:ARG:HA	3:H:83:ARG:HE	1.80	0.46
1:L:8:LYS:O	1:L:11:VAL:HG11	2.14	0.46
1:L:69:PRO:CB	1:L:78:ALA:HB3	2.46	0.46
1:L:69:PRO:HA	1:L:82:LYS:HD3	1.97	0.46
1:L:70:ALA:H	1:L:82:LYS:HD3	1.80	0.46
1:L:100:TRP:O	1:L:103:ARG:N	2.49	0.46
1:L:110:LYS:HE2	2:M:254:TRP:HZ3	1.81	0.46
1:L:127:ALA:HB3	4:L:283:BCL:H52	1.96	0.46
1:L:171:PRO:C	1:L:173:HIS:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:72:ILE:HD13	2:M:72:ILE:HA	1.63	0.46
2:M:204:LEU:C	2:M:206:ILE:N	2.66	0.46
2:M:209:LEU:HA	2:M:276:VAL:HG21	1.97	0.46
3:H:151:LEU:HA	3:H:152:PRO:HD2	1.75	0.46
1:L:146:PHE:CB	1:L:156:TRP:CG	2.96	0.46
2:M:168:MET:CG	2:M:173:GLU:HG3	2.45	0.46
2:M:70:ILE:CD1	2:M:74:PHE:CD2	2.99	0.46
2:M:206:ILE:HG21	4:M:311:BCL:C2D	2.45	0.46
1:L:124:ALA:CB	5:L:284:BPH:HBC2	2.42	0.46
1:L:185:LEU:CA	1:L:188:ALA:H	2.28	0.46
1:L:193:LEU:O	1:L:194:VAL:C	2.54	0.46
1:L:249:ILE:HG22	1:L:250:ILE:N	2.31	0.46
4:L:282:BCL:C2	5:M:312:BPH:HMB2	2.46	0.46
5:L:284:BPH:OBB	5:L:284:BPH:CHC	2.64	0.46
2:M:7:PHE:CD1	2:M:7:PHE:O	2.69	0.46
2:M:165:PRO:CB	2:M:173:GLU:HB2	2.46	0.46
2:M:168:MET:HE1	2:M:288:GLY:HA3	1.96	0.46
2:M:186:THR:HG22	4:M:310:BCL:HHD	1.97	0.46
2:M:278:LEU:C	2:M:278:LEU:HD12	2.36	0.46
1:L:97:PHE:CE1	4:L:283:BCL:C13	2.96	0.46
1:L:128:TYR:CD1	1:L:129:LEU:N	2.84	0.46
1:L:226:THR:HG22	2:M:232:GLU:HB2	1.91	0.46
1:L:249:ILE:HG23	1:L:249:ILE:O	2.15	0.46
2:M:37:THR:HA	2:M:41:TRP:NE1	2.31	0.46
2:M:150:PHE:CD1	5:M:312:BPH:C3D	2.99	0.46
2:M:164:ARG:HG2	2:M:164:ARG:NH1	2.28	0.46
3:H:118:ARG:HH11	3:H:227:LEU:HD12	1.79	0.46
1:L:194:VAL:HG21	2:M:234:GLU:OE1	2.16	0.45
4:L:283:BCL:H8	4:M:311:BCL:CBB	2.46	0.45
2:M:24:VAL:O	2:M:26:LEU:HB3	2.16	0.45
4:M:311:BCL:HBB3	4:M:311:BCL:CMB	2.42	0.45
3:H:40:TYR:N	3:H:42:LEU:HD11	2.24	0.45
3:H:157:ASP:CG	3:H:211:ASP:OD1	2.53	0.45
3:H:204:HIS:CE1	3:H:213:PHE:CE2	3.04	0.45
1:L:68:PRO:HB2	1:L:69:PRO:CD	2.46	0.45
2:M:28:ASN:O	2:M:30:SER:O	2.34	0.45
2:M:155:TRP:C	2:M:157:TRP:N	2.68	0.45
2:M:201:PHE:CE2	2:M:282:ILE:CG2	2.99	0.45
2:M:273:ALA:O	2:M:276:VAL:HB	2.16	0.45
1:L:9:TYR:CE2	2:M:243:THR:HG23	2.52	0.45
1:L:48:LEU:CG	1:L:89:ILE:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:LEU:O	1:L:158:SER:HB2	2.16	0.45
1:L:248:MET:HE2	4:L:283:BCL:OBD	2.16	0.45
2:M:65:MET:CG	2:M:66:TRP:H	2.26	0.45
2:M:256:MET:CE	6:M:313:U10:H102	2.45	0.45
3:H:27:LEU:O	3:H:28:ILE:O	2.35	0.45
3:H:94:GLU:O	3:H:96:PHE:CA	2.62	0.45
3:H:96:PHE:CD1	3:H:97:PRO:HD2	2.52	0.45
3:H:117:ARG:NH1	3:H:231:ASP:OD1	2.49	0.45
3:H:191:LEU:HD22	3:H:205:VAL:HG21	1.98	0.45
1:L:128:TYR:C	1:L:130:THR:N	2.69	0.45
1:L:204:LYS:CD	1:L:207:ARG:HH22	2.23	0.45
1:L:216:PHE:HD1	1:L:216:PHE:HA	1.54	0.45
2:M:46:GLN:HE21	2:M:49:PRO:CD	2.08	0.45
2:M:62:SER:C	2:M:64:LEU:N	2.70	0.45
2:M:87:ARG:C	2:M:89:LEU:H	2.19	0.45
2:M:218:MET:HE1	6:M:313:U10:C1M	2.47	0.45
2:M:259:ASN:C	2:M:259:ASN:ND2	2.70	0.45
2:M:264:GLY:HA2	2:M:267:ARG:CG	2.45	0.45
3:H:17:ILE:HD11	3:H:21:TRP:HE1	1.80	0.45
3:H:32:GLN:O	3:H:34:GLU:N	2.49	0.45
3:H:204:HIS:CD2	3:H:206:ASN:N	2.84	0.45
3:H:204:HIS:HE1	3:H:213:PHE:HZ	1.63	0.45
1:L:8:LYS:C	3:H:87:LEU:CD2	2.85	0.45
1:L:84:GLY:CA	1:L:87:GLN:HB2	2.47	0.45
1:L:193:LEU:C	1:L:195:LEU:N	2.68	0.45
1:L:249:ILE:CG2	1:L:250:ILE:N	2.78	0.45
2:M:90:PHE:CB	2:M:179:ILE:HD12	2.47	0.45
2:M:109:LEU:O	2:M:113:GLY:HA3	2.17	0.45
2:M:185:TRP:CZ3	2:M:186:THR:HA	2.52	0.45
3:H:37:ARG:NH2	3:H:44:ASN:OD1	2.48	0.45
1:L:86:TRP:CE3	1:L:87:GLN:HA	2.50	0.45
1:L:11:VAL:O	1:L:12:PRO:C	2.55	0.45
1:L:124:ALA:O	1:L:127:ALA:N	2.50	0.45
1:L:170:ASN:C	1:L:170:ASN:OD1	2.55	0.45
1:L:182:THR:O	1:L:186:ALA:CB	2.65	0.45
2:M:72:ILE:O	2:M:72:ILE:HD12	2.16	0.45
1:L:170:ASN:ND2	1:L:247:CYS:O	2.49	0.45
1:L:193:LEU:HD23	6:L:285:U10:O3	2.14	0.45
4:L:283:BCL:C4	5:L:284:BPH:OBB	2.64	0.45
2:M:152:SER:CA	2:M:277:THR:HG22	2.42	0.45
2:M:192:VAL:HG12	2:M:192:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:218:MET:HE1	6:M:313:U10:H1M3	1.98	0.45
2:M:252:TRP:CD1	6:M:313:U10:C6	2.99	0.45
3:H:168:TRP:CH2	3:H:223:THR:C	2.91	0.45
1:L:54:VAL:C	1:L:56:GLN:H	2.20	0.45
1:L:90:THR:C	1:L:92:CYS:N	2.70	0.45
1:L:177:ILE:HD12	4:L:283:BCL:HMB3	1.99	0.45
2:M:62:SER:O	2:M:64:LEU:N	2.50	0.45
2:M:208:PHE:C	2:M:276:VAL:HG22	2.30	0.45
2:M:237:GLN:O	2:M:239:ALA:N	2.50	0.45
3:H:130:LYS:O	3:H:171:ILE:CD1	2.57	0.45
3:H:179:LEU:HD21	3:H:181:VAL:CG2	2.46	0.45
1:L:93:ALA:HB1	1:L:97:PHE:HE2	1.75	0.45
1:L:109:ARG:HA	1:L:109:ARG:NE	2.31	0.45
2:M:44:ASN:HD22	2:M:44:ASN:HA	1.42	0.45
2:M:152:SER:HA	2:M:277:THR:CG2	2.46	0.45
3:H:131:ILE:HD11	3:H:225:VAL:CG2	2.47	0.45
1:L:147:PRO:CG	1:L:152:THR:CG2	2.92	0.44
1:L:156:TRP:HZ3	1:L:157:VAL:HA	1.75	0.44
1:L:185:LEU:O	1:L:188:ALA:CA	2.61	0.44
1:L:241:VAL:HG21	5:L:284:BPH:CBC	2.46	0.44
1:L:268:LYS:HB3	1:L:268:LYS:HE2	1.43	0.44
2:M:55:LEU:O	2:M:57:VAL:N	2.50	0.44
2:M:92:PHE:O	2:M:93:SER:CB	2.62	0.44
2:M:133:THR:HG21	2:M:146:THR:HG21	2.00	0.44
2:M:191:LEU:N	2:M:191:LEU:CD1	2.80	0.44
2:M:258:PHE:CD1	2:M:258:PHE:C	2.89	0.44
2:M:284:ILE:O	2:M:284:ILE:HG23	2.17	0.44
3:H:24:LEU:HD23	3:H:28:ILE:HD12	1.87	0.44
1:L:102:LEU:O	1:L:104:GLU:N	2.51	0.44
1:L:146:PHE:HA	1:L:156:TRP:CD1	2.53	0.44
4:M:310:BCL:H41	5:M:312:BPH:HBB2	1.98	0.44
3:H:130:LYS:HZ3	3:H:131:ILE:HG22	1.83	0.44
1:L:16:LEU:HB2	1:L:106:GLU:OE2	2.17	0.44
1:L:47:ILE:O	1:L:49:ILE:N	2.50	0.44
1:L:123:PHE:CG	1:L:238:LEU:CD2	2.96	0.44
1:L:147:PRO:CG	1:L:156:TRP:HB2	2.47	0.44
1:L:183:ASN:HA	1:L:186:ALA:HB3	1.98	0.44
2:M:212:SER:O	2:M:215:LEU:N	2.51	0.44
2:M:297:TRP:O	2:M:301:HIS:HD2	2.01	0.44
3:H:213:PHE:CD1	3:H:216:ILE:HD11	2.52	0.44
1:L:244:SER:HB3	4:L:283:BCL:HBA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:285:U10:H3M3	6:L:285:U10:C4M	2.47	0.44
2:M:11:GLN:NE2	3:H:144:ALA:CB	2.79	0.44
2:M:35:PHE:CD2	2:M:47:LEU:HD12	2.39	0.44
2:M:58:LEU:O	2:M:62:SER:N	2.51	0.44
2:M:105:PHE:CD1	2:M:106:ALA:CB	3.01	0.44
2:M:109:LEU:HD22	2:M:110:LYS:HA	1.98	0.44
1:L:5:PHE:CZ	3:H:40:TYR:CZ	2.91	0.44
1:L:17:VAL:C	1:L:19:GLY:H	2.20	0.44
1:L:102:LEU:C	1:L:104:GLU:N	2.68	0.44
2:M:77:GLN:HE21	2:M:77:GLN:HB2	1.54	0.44
2:M:93:SER:HB2	2:M:178:GLY:CA	2.44	0.44
2:M:148:TRP:C	2:M:150:PHE:H	2.12	0.44
4:M:310:BCL:H42	5:M:312:BPH:HBB2	1.98	0.44
3:H:83:ARG:HA	3:H:84:PRO:HD2	1.78	0.44
3:H:100:PRO:HB3	3:H:109:VAL:HG11	1.99	0.44
3:H:135:LYS:C	3:H:137:ALA:H	2.20	0.44
3:H:143:SER:O	3:H:144:ALA:O	2.35	0.44
1:L:69:PRO:HG2	1:L:78:ALA:HB3	1.96	0.44
1:L:87:GLN:O	1:L:90:THR:HB	2.18	0.44
1:L:150:ILE:HG22	1:L:151:TRP:CD1	2.53	0.44
1:L:200:PRO:HB2	1:L:201:GLU:H	1.63	0.44
1:L:232:LEU:CB	2:M:42:PHE:HZ	2.30	0.44
2:M:35:PHE:CB	2:M:39:LEU:CD2	2.95	0.44
1:L:6:GLU:C	1:L:8:LYS:N	2.70	0.44
1:L:175:ILE:CG2	1:L:179:PHE:CE1	3.00	0.44
1:L:177:ILE:HG21	1:L:181:PHE:HE2	1.80	0.44
6:L:285:U10:H321	2:M:60:LEU:HD21	1.99	0.44
2:M:51:TYR:CE1	2:M:53:GLY:CA	3.00	0.44
2:M:81:ASN:O	2:M:82:PRO:C	2.56	0.44
6:M:313:U10:H33	6:M:313:U10:H372	1.74	0.44
3:H:18:TYR:CD1	3:H:18:TYR:C	2.90	0.44
3:H:36:MET:HE3	3:H:36:MET:HB2	1.56	0.44
3:H:57:PRO:C	3:H:58:LEU:HD12	2.37	0.44
1:L:84:GLY:O	1:L:86:TRP:C	2.56	0.44
1:L:102:LEU:N	1:L:102:LEU:HD22	2.30	0.44
1:L:190:HIS:CE1	1:L:229:ILE:HG21	2.52	0.44
2:M:58:LEU:O	2:M:60:LEU:N	2.51	0.44
1:L:10:ARG:NH2	3:H:95:GLY:O	2.51	0.44
1:L:10:ARG:CZ	1:L:25:TRP:CG	3.01	0.44
1:L:98:VAL:HG23	1:L:125:ILE:CD1	2.47	0.44
1:L:112:GLY:HA3	2:M:247:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:LEU:HD13	1:L:146:PHE:HE2	1.83	0.44
1:L:161:GLY:O	1:L:163:THR:N	2.51	0.44
2:M:244:ALA:O	2:M:245:ALA:O	2.36	0.44
2:M:265:ILE:O	2:M:268:TRP:HB2	2.18	0.44
2:M:282:ILE:HG22	2:M:283:GLY:N	2.32	0.44
5:M:312:BPH:H2A	5:M:312:BPH:O2D	2.17	0.44
3:H:27:LEU:HD12	3:H:28:ILE:CA	2.33	0.44
1:L:242:PHE:C	1:L:244:SER:N	2.71	0.43
2:M:124:VAL:O	2:M:125:ALA:O	2.36	0.43
3:H:105:MET:CB	3:H:106:LYS:HZ3	2.30	0.43
3:H:219:ILE:HG21	3:H:225:VAL:HG12	1.99	0.43
1:L:105:VAL:O	1:L:107:ILE:N	2.51	0.43
2:M:35:PHE:CE1	2:M:38:LEU:HD22	2.54	0.43
2:M:41:TRP:HA	2:M:41:TRP:CE3	2.53	0.43
2:M:163:ILE:HG21	2:M:285:LEU:CD1	2.44	0.43
2:M:222:THR:C	2:M:224:LEU:N	2.71	0.43
3:H:158:LEU:HD12	3:H:158:LEU:HA	1.77	0.43
3:H:227:LEU:O	3:H:228:LEU:C	2.56	0.43
1:L:48:LEU:HD13	1:L:85:LEU:HA	2.00	0.43
1:L:68:PRO:HB3	1:L:86:TRP:CZ2	2.52	0.43
1:L:110:LYS:C	1:L:112:GLY:N	2.70	0.43
1:L:113:ILE:CD1	2:M:225:ALA:O	2.64	0.43
1:L:177:ILE:HD11	4:L:283:BCL:C1B	2.47	0.43
1:L:225:GLY:HA2	6:L:285:U10:H4M2	1.97	0.43
5:L:284:BPH:CMC	2:M:213:ALA:HB1	2.49	0.43
2:M:165:PRO:HG3	2:M:173:GLU:CB	2.48	0.43
2:M:205:SER:N	2:M:279:THR:CG2	2.80	0.43
3:H:88:ALA:C	3:H:89:ARG:HG2	2.38	0.43
3:H:102:GLY:O	3:H:103:ASP:C	2.57	0.43
3:H:140:PHE:CE2	3:H:169:VAL:HG11	2.50	0.43
1:L:6:GLU:C	1:L:8:LYS:H	2.22	0.43
1:L:79:PRO:HG2	1:L:82:LYS:H	1.84	0.43
1:L:123:PHE:CD2	1:L:238:LEU:HD23	2.53	0.43
2:M:60:LEU:O	2:M:61:PHE:C	2.56	0.43
2:M:73:TRP:CH2	2:M:109:LEU:CD2	3.00	0.43
2:M:150:PHE:CD1	5:M:312:BPH:C2D	3.01	0.43
2:M:201:PHE:CZ	2:M:282:ILE:HG21	2.53	0.43
3:H:85:ILE:H	3:H:85:ILE:HG12	1.49	0.43
3:H:171:ILE:CD1	3:H:171:ILE:H	2.30	0.43
1:L:8:LYS:NZ	1:L:9:TYR:HE1	2.14	0.43
1:L:116:HIS:CE1	2:M:225:ALA:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:159:ASN:O	1:L:162:TYR:N	2.52	0.43
1:L:178:SER:O	1:L:182:THR:HB	2.18	0.43
2:M:69:THR:CG2	2:M:118:ALA:HB2	2.49	0.43
2:M:87:ARG:HG3	2:M:88:ASP:CG	2.38	0.43
2:M:113:GLY:O	2:M:116:LEU:N	2.52	0.43
2:M:119:SER:CB	2:M:177:TYR:CE2	3.02	0.43
2:M:268:TRP:HA	2:M:268:TRP:CE3	2.54	0.43
3:H:149:ILE:C	3:H:151:LEU:N	2.72	0.43
3:H:170:ASP:OD2	3:H:177:ARG:NE	2.52	0.43
1:L:69:PRO:HA	1:L:82:LYS:CD	2.48	0.43
1:L:135:ARG:N	1:L:136:PRO:HD2	2.33	0.43
1:L:147:PRO:CD	1:L:156:TRP:CD1	3.01	0.43
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.99	0.43
1:L:231:ARG:NH2	2:M:7:PHE:CB	2.82	0.43
1:L:237:SER:HB2	2:M:213:ALA:O	2.18	0.43
2:M:69:THR:O	2:M:72:ILE:HG22	2.18	0.43
2:M:122:MET:O	2:M:126:VAL:CG2	2.66	0.43
3:H:116:ALA:HB1	3:H:228:LEU:CD1	2.48	0.43
3:H:148:PRO:O	3:H:151:LEU:N	2.48	0.43
3:H:190:LEU:HD22	3:H:219:ILE:HD11	2.00	0.43
1:L:11:VAL:HA	1:L:12:PRO:HD2	1.62	0.43
1:L:54:VAL:O	1:L:55:LEU:C	2.56	0.43
1:L:138:MET:SD	1:L:249:ILE:HD11	2.59	0.43
2:M:12:VAL:HG22	3:H:141:HIS:O	2.18	0.43
2:M:36:SER:O	2:M:40:GLY:HA3	2.18	0.43
2:M:58:LEU:C	2:M:60:LEU:N	2.71	0.43
3:H:210:SER:O	3:H:212:LEU:CA	2.63	0.43
1:L:72:GLU:OE2	1:L:72:GLU:C	2.56	0.43
1:L:178:SER:CB	4:L:282:BCL:O1A	2.42	0.43
2:M:26:LEU:CG	2:M:27:ALA:N	2.81	0.43
2:M:76:TYR:C	2:M:76:TYR:CD1	2.93	0.43
2:M:119:SER:HA	2:M:177:TYR:CZ	2.50	0.43
2:M:237:GLN:C	2:M:239:ALA:N	2.71	0.43
3:H:20:PHE:CD1	3:H:21:TRP:N	2.81	0.43
3:H:168:TRP:CH2	3:H:224:GLU:N	2.87	0.43
1:L:9:TYR:O	1:L:11:VAL:HG22	2.19	0.43
1:L:31:VAL:HG13	6:M:313:U10:C40	2.49	0.43
1:L:111:LEU:CD2	2:M:251:PHE:CB	2.93	0.43
1:L:167:PHE:CE2	4:L:283:BCL:C2D	3.01	0.43
2:M:96:PRO:O	2:M:98:ALA:N	2.50	0.43
3:H:134:MET:SD	3:H:141:HIS:HE1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:196:VAL:HA	3:H:205:VAL:N	2.32	0.43
3:H:242:MET:HE3	3:H:243:TYR:CZ	2.54	0.43
1:L:26:VAL:O	1:L:27:GLY:C	2.57	0.43
1:L:219:LEU:HA	1:L:219:LEU:HD12	1.82	0.43
4:L:282:BCL:H2C	4:L:282:BCL:HBC3	1.50	0.43
2:M:264:GLY:C	2:M:267:ARG:H	2.21	0.43
3:H:58:LEU:N	3:H:58:LEU:HD12	2.34	0.43
3:H:65:ILE:CG2	3:H:65:ILE:O	2.66	0.43
3:H:106:LYS:HB2	3:H:106:LYS:HE2	1.43	0.43
1:L:11:VAL:O	1:L:11:VAL:HG23	2.18	0.42
1:L:101:ALA:HB2	1:L:121:PHE:CE1	2.47	0.42
1:L:135:ARG:C	1:L:139:MET:HE3	2.39	0.42
1:L:185:LEU:HD23	1:L:186:ALA:H	0.48	0.42
1:L:248:MET:HA	1:L:251:THR:HG22	2.00	0.42
2:M:24:VAL:O	2:M:24:VAL:CG1	2.67	0.42
2:M:116:LEU:HA	2:M:116:LEU:HD23	1.78	0.42
2:M:214:LEU:O	2:M:217:ALA:CA	2.67	0.42
1:L:147:PRO:HD3	1:L:156:TRP:HD1	1.83	0.42
1:L:148:TYR:HD1	1:L:148:TYR:HA	1.69	0.42
1:L:262:TRP:C	1:L:264:GLN:H	2.19	0.42
5:L:284:BPH:H3A	5:L:284:BPH:HBA1	1.73	0.42
2:M:209:LEU:HG	4:M:310:BCL:O1A	2.20	0.42
2:M:285:LEU:HD23	2:M:285:LEU:H	1.85	0.42
5:M:312:BPH:C6	5:M:312:BPH:H8	2.46	0.42
3:H:39:GLY:HA2	3:H:42:LEU:HD11	2.00	0.42
1:L:51:TRP:HH2	1:L:80:LEU:CD1	2.32	0.42
1:L:166:ASN:C	1:L:166:ASN:OD1	2.57	0.42
1:L:210:ASP:OD1	1:L:213:ASP:HB2	2.19	0.42
1:L:249:ILE:O	1:L:249:ILE:HD13	2.19	0.42
5:L:284:BPH:HHD	5:L:284:BPH:HMD1	1.86	0.42
2:M:87:ARG:NH1	2:M:87:ARG:HB2	2.34	0.42
2:M:208:PHE:CB	2:M:276:VAL:HG22	2.47	0.42
3:H:151:LEU:HD22	3:H:202:ARG:C	2.39	0.42
3:H:229:GLU:O	3:H:233:ILE:CD1	2.67	0.42
1:L:49:ILE:CB	1:L:89:ILE:HD11	2.49	0.42
1:L:167:PHE:HD2	4:L:283:BCL:HHD	1.76	0.42
4:L:283:BCL:OBB	4:L:283:BCL:HHC	2.19	0.42
2:M:157:TRP:O	2:M:158:MET:C	2.58	0.42
2:M:160:LEU:HD21	4:M:310:BCL:OBD	2.20	0.42
2:M:242:GLY:HA3	3:H:117:ARG:HD3	2.01	0.42
2:M:279:THR:O	2:M:282:ILE:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:308:BOG:H2'2	7:M:308:BOG:H5'1	1.22	0.42
3:H:196:VAL:N	3:H:205:VAL:HA	2.35	0.42
1:L:75:LEU:HD23	1:L:141:ALA:HA	2.01	0.42
1:L:91:ILE:HG22	1:L:91:ILE:O	2.19	0.42
1:L:97:PHE:CE1	4:L:283:BCL:H143	2.38	0.42
1:L:139:MET:C	1:L:141:ALA:N	2.72	0.42
1:L:246:LEU:O	1:L:247:CYS:C	2.57	0.42
4:L:282:BCL:HHC	4:L:282:BCL:CBB	2.41	0.42
2:M:56:GLY:CA	2:M:132:ARG:HD2	2.49	0.42
2:M:110:LYS:HA	2:M:110:LYS:HD3	1.32	0.42
2:M:137:ALA:O	2:M:141:GLY:N	2.52	0.42
3:H:105:MET:H	3:H:106:LYS:NZ	2.14	0.42
3:H:116:ALA:CA	3:H:228:LEU:HD11	2.43	0.42
1:L:9:TYR:CD1	2:M:250:LEU:HD11	2.55	0.42
1:L:123:PHE:CE2	1:L:238:LEU:CD2	3.03	0.42
1:L:157:VAL:HG12	1:L:158:SER:N	2.35	0.42
4:L:283:BCL:H72	4:M:311:BCL:CBB	2.50	0.42
2:M:60:LEU:O	2:M:64:LEU:HD13	2.18	0.42
2:M:115:TRP:CE3	2:M:116:LEU:N	2.87	0.42
2:M:224:LEU:C	2:M:226:VAL:N	2.69	0.42
2:M:271:TRP:CH2	3:H:31:LEU:CD2	3.02	0.42
2:M:290:VAL:HG21	3:H:12:LEU:HD13	2.01	0.42
3:H:153:VAL:O	3:H:153:VAL:HG12	2.19	0.42
1:L:135:ARG:NH1	1:L:139:MET:SD	2.92	0.42
1:L:150:ILE:CD1	1:L:150:ILE:H	2.33	0.42
6:L:285:U10:H271	6:L:285:U10:H251	1.67	0.42
2:M:35:PHE:CB	2:M:39:LEU:HD22	2.49	0.42
2:M:73:TRP:CZ2	2:M:114:LEU:HD11	2.55	0.42
2:M:130:TRP:HZ3	2:M:147:ALA:O	2.02	0.42
2:M:163:ILE:HG22	2:M:164:ARG:N	2.35	0.42
2:M:208:PHE:HB2	2:M:276:VAL:CG2	2.50	0.42
2:M:266:HIS:HA	2:M:269:ALA:CB	2.50	0.42
3:H:26:GLY:O	3:H:30:TYR:CB	2.64	0.42
3:H:60:LYS:HD2	3:H:62:LYS:HG2	2.00	0.42
3:H:184:LYS:HE2	3:H:186:GLY:HA2	2.01	0.42
3:H:193:MET:C	3:H:195:MET:N	2.72	0.42
1:L:6:GLU:HG2	1:L:10:ARG:CD	2.50	0.42
1:L:111:LEU:HD22	2:M:251:PHE:HA	2.01	0.42
1:L:177:ILE:O	1:L:181:PHE:N	2.52	0.42
4:L:282:BCL:H2	5:M:312:BPH:C2B	2.50	0.42
3:H:111:PRO:CD	3:H:243:TYR:CZ	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:PHE:CE1	2:M:246:GLU:HA	2.54	0.42
1:L:8:LYS:O	3:H:87:LEU:HD21	2.20	0.42
1:L:60:ASN:O	1:L:62:GLN:CA	2.67	0.42
1:L:127:ALA:HB3	4:L:283:BCL:C2	2.46	0.42
1:L:174:MET:SD	4:L:282:BCL:O1D	2.78	0.42
1:L:179:PHE:HB3	1:L:236:LEU:O	2.20	0.42
1:L:231:ARG:HH22	2:M:7:PHE:HA	1.69	0.42
1:L:255:TRP:CZ2	1:L:262:TRP:HE3	2.38	0.42
1:L:263:TRP:CG	2:M:180:PHE:HE2	2.34	0.42
2:M:59:SER:O	2:M:63:GLY:N	2.47	0.42
2:M:279:THR:CG2	2:M:280:GLY:N	2.82	0.42
4:M:310:BCL:H172	5:M:312:BPH:CMB	2.50	0.42
3:H:64:PHE:HB2	3:H:73:LEU:O	2.19	0.42
3:H:83:ARG:HA	3:H:83:ARG:NE	2.35	0.42
3:H:43:GLU:CD	3:H:44:ASN:HD21	2.23	0.42
3:H:182:GLU:HA	3:H:188:THR:HA	2.02	0.42
3:H:195:MET:O	3:H:196:VAL:O	2.38	0.42
1:L:185:LEU:N	1:L:185:LEU:HD22	2.35	0.41
1:L:189:LEU:HD22	1:L:216:PHE:HZ	1.85	0.41
2:M:35:PHE:CE2	2:M:39:LEU:HD21	2.55	0.41
2:M:73:TRP:CD2	2:M:114:LEU:HD21	2.55	0.41
3:H:143:SER:O	3:H:143:SER:OG	2.35	0.41
3:H:201:ASN:OD1	3:H:202:ARG:CB	2.68	0.41
1:L:113:ILE:CG2	2:M:225:ALA:HB1	2.49	0.41
1:L:121:PHE:HB2	5:L:284:BPH:C3D	2.50	0.41
1:L:240:ALA:O	1:L:241:VAL:C	2.58	0.41
2:M:15:PRO:HD2	3:H:140:PHE:CD1	2.52	0.41
2:M:238:ILE:CD1	2:M:263:GLU:HG3	2.50	0.41
1:L:109:ARG:HE	1:L:109:ARG:N	2.19	0.41
2:M:152:SER:OG	2:M:277:THR:HG22	2.20	0.41
3:H:17:ILE:O	3:H:21:TRP:HD1	2.03	0.41
3:H:37:ARG:O	3:H:42:LEU:HD12	2.19	0.41
3:H:190:LEU:HD11	3:H:225:VAL:HG11	2.02	0.41
1:L:123:PHE:O	1:L:127:ALA:N	2.53	0.41
1:L:205:GLU:HG3	3:H:67:PRO:HA	2.01	0.41
2:M:191:LEU:HD13	2:M:191:LEU:N	2.35	0.41
2:M:211:GLY:O	2:M:214:LEU:HB3	2.20	0.41
2:M:279:THR:O	2:M:281:GLY:N	2.53	0.41
1:L:9:TYR:HE2	2:M:243:THR:HG23	1.85	0.41
1:L:146:PHE:HE1	1:L:148:TYR:HE1	1.68	0.41
1:L:168:HIS:HE1	2:M:183:LEU:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:221:GLY:HA3	2:M:50:ILE:HG13	2.01	0.41
2:M:130:TRP:CZ3	2:M:147:ALA:O	2.73	0.41
3:H:17:ILE:HD11	3:H:21:TRP:NE1	2.35	0.41
3:H:90:THR:OG1	3:H:97:PRO:O	2.38	0.41
3:H:121:PRO:HG3	3:H:224:GLU:HG2	2.02	0.41
3:H:130:LYS:HG2	3:H:172:PRO:HG2	2.02	0.41
1:L:86:TRP:HZ2	1:L:145:ALA:CB	2.33	0.41
2:M:16:ALA:HB2	2:M:32:VAL:HG21	1.96	0.41
2:M:27:ALA:HB1	2:M:52:LEU:H	1.86	0.41
2:M:35:PHE:HB3	2:M:39:LEU:HD22	2.02	0.41
2:M:152:SER:OG	2:M:274:VAL:HG22	2.20	0.41
2:M:164:ARG:CB	2:M:165:PRO:CD	2.69	0.41
2:M:228:ARG:HH22	3:H:241:LEU:HD21	1.84	0.41
3:H:234:CYS:O	3:H:237:VAL:CG2	2.61	0.41
1:L:37:ALA:C	1:L:39:PHE:N	2.72	0.41
1:L:126:LEU:O	1:L:126:LEU:HD13	2.21	0.41
1:L:146:PHE:C	1:L:146:PHE:HD1	2.23	0.41
1:L:193:LEU:CD2	6:L:285:U10:C2	2.98	0.41
1:L:244:SER:CB	4:L:283:BCL:HBA2	2.51	0.41
2:M:64:LEU:O	2:M:65:MET:C	2.58	0.41
2:M:94:LEU:HD11	2:M:114:LEU:CB	2.50	0.41
2:M:290:VAL:HG12	3:H:13:ALA:HB2	2.03	0.41
3:H:134:MET:HB3	3:H:166:ASP:OD2	2.21	0.41
3:H:155:GLY:CA	3:H:204:HIS:CD2	3.04	0.41
3:H:168:TRP:CZ3	3:H:223:THR:O	2.74	0.41
3:H:234:CYS:C	3:H:237:VAL:CG2	2.89	0.41
1:L:29:PHE:N	1:L:29:PHE:CD1	2.89	0.41
1:L:73:TYR:CB	1:L:82:LYS:HZ2	2.32	0.41
1:L:160:THR:O	1:L:164:TYR:CD1	2.72	0.41
1:L:173:HIS:CE1	1:L:177:ILE:CD1	2.90	0.41
2:M:113:GLY:O	2:M:114:LEU:O	2.39	0.41
2:M:159:VAL:C	2:M:161:GLY:H	2.21	0.41
1:L:60:ASN:CG	1:L:63:LEU:HD12	2.41	0.41
1:L:69:PRO:HG3	1:L:78:ALA:HB3	1.98	0.41
1:L:87:GLN:O	1:L:88:ILE:C	2.60	0.41
1:L:111:LEU:CD2	2:M:251:PHE:HA	2.51	0.41
1:L:127:ALA:O	1:L:130:THR:HB	2.20	0.41
1:L:146:PHE:C	1:L:146:PHE:CD1	2.93	0.41
1:L:159:ASN:O	1:L:161:GLY:N	2.54	0.41
1:L:187:LEU:HA	1:L:187:LEU:HD13	1.88	0.41
1:L:187:LEU:CA	2:M:216:PHE:CE2	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:215:PHE:HD1	1:L:216:PHE:CD1	2.39	0.41
1:L:269:LEU:CD1	1:L:270:PRO:CD	2.90	0.41
4:L:283:BCL:C2C	4:M:310:BCL:CBC	2.85	0.41
2:M:14:GLY:HA3	3:H:140:PHE:CD1	2.55	0.41
2:M:201:PHE:HB2	2:M:283:GLY:HA2	2.03	0.41
2:M:252:TRP:CD1	6:M:313:U10:C1	3.04	0.41
2:M:256:MET:HE1	6:M:313:U10:H102	2.02	0.41
2:M:263:GLU:O	2:M:266:HIS:N	2.49	0.41
3:H:117:ARG:CB	3:H:227:LEU:HB3	2.43	0.41
3:H:218:THR:CG2	3:H:219:ILE:N	2.83	0.41
1:L:15:THR:HG21	1:L:19:GLY:C	2.40	0.41
1:L:32:GLY:C	1:L:34:PHE:H	2.20	0.41
1:L:61:PRO:O	1:L:64:ILE:HG23	2.21	0.41
2:M:20:MET:CG	2:M:22:GLU:N	2.70	0.41
2:M:21:THR:OG1	2:M:23:ASP:CA	2.69	0.41
2:M:165:PRO:HB3	2:M:173:GLU:HB2	2.02	0.41
3:H:155:GLY:HA3	3:H:210:SER:H	1.86	0.41
1:L:149:GLY:O	1:L:152:THR:N	2.54	0.40
2:M:152:SER:HB3	2:M:277:THR:HG21	2.03	0.40
6:M:313:U10:H252	6:M:313:U10:H212	1.64	0.40
3:H:109:VAL:O	3:H:112:ALA:HB3	2.20	0.40
3:H:166:ASP:O	3:H:179:LEU:HA	2.22	0.40
1:L:170:ASN:HB2	1:L:259:TRP:CD1	2.53	0.40
2:M:65:MET:O	2:M:66:TRP:C	2.59	0.40
2:M:260:ALA:CB	3:H:36:MET:SD	3.08	0.40
2:M:275:LEU:O	2:M:276:VAL:C	2.59	0.40
2:M:279:THR:HG22	2:M:280:GLY:H	1.86	0.40
3:H:108:GLY:HA3	3:H:114:TRP:CE3	2.54	0.40
3:H:189:ARG:HB3	3:H:189:ARG:NH1	2.09	0.40
1:L:55:LEU:HA	1:L:55:LEU:HD23	1.56	0.40
1:L:110:LYS:HE3	2:M:254:TRP:CH2	2.56	0.40
1:L:176:ALA:HB2	1:L:243:PHE:HB3	2.02	0.40
1:L:206:MET:HB2	3:H:65:ILE:O	2.19	0.40
1:L:235:LEU:HD22	1:L:235:LEU:HA	1.87	0.40
2:M:168:MET:HG3	2:M:173:GLU:CD	2.42	0.40
3:H:179:LEU:CD2	3:H:181:VAL:HG21	2.50	0.40
3:H:226:THR:O	3:H:229:GLU:HB2	2.21	0.40
1:L:49:ILE:C	1:L:51:TRP:N	2.74	0.40
1:L:84:GLY:HA2	1:L:87:GLN:HB2	2.03	0.40
1:L:122:ALA:O	1:L:126:LEU:HB2	2.21	0.40
1:L:185:LEU:HD23	1:L:185:LEU:N	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:37:THR:O	2:M:38:LEU:O	2.39	0.40
2:M:105:PHE:CD1	2:M:105:PHE:N	2.86	0.40
2:M:130:TRP:HE3	2:M:150:PHE:HD2	1.68	0.40
2:M:152:SER:CB	2:M:277:THR:HG21	2.50	0.40
2:M:164:ARG:O	2:M:167:LEU:CB	2.65	0.40
2:M:170:SER:O	2:M:173:GLU:HB2	2.21	0.40
2:M:233:ARG:HH11	2:M:233:ARG:HD3	1.65	0.40
4:M:310:BCL:H61	5:M:312:BPH:HBB2	2.03	0.40
5:M:312:BPH:C10	5:M:312:BPH:C12	2.83	0.40
3:H:147:ASN:HA	3:H:148:PRO:HD2	1.86	0.40
3:H:183:LEU:CG	3:H:189:ARG:NE	2.83	0.40
3:H:185:ASP:O	3:H:186:GLY:C	2.60	0.40
1:L:5:PHE:HB2	1:L:8:LYS:HZ1	1.87	0.40
1:L:84:GLY:HA2	1:L:87:GLN:CB	2.51	0.40
1:L:101:ALA:C	1:L:104:GLU:H	2.25	0.40
1:L:146:PHE:CE1	1:L:148:TYR:HE1	2.39	0.40
2:M:21:THR:HG22	2:M:140:LEU:HD12	2.00	0.40
2:M:94:LEU:HD21	2:M:115:TRP:N	2.36	0.40
2:M:130:TRP:CH2	2:M:151:LEU:HD11	2.56	0.40
3:H:37:ARG:O	3:H:38:GLU:C	2.59	0.40
3:H:117:ARG:H	3:H:117:ARG:HG2	1.52	0.40
3:H:130:LYS:NZ	3:H:130:LYS:CB	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	264/281 (94%)	118 (45%)	65 (25%)	81 (31%)	0 0
2	M	294/307 (96%)	141 (48%)	74 (25%)	79 (27%)	0 0
3	H	235/260 (90%)	107 (46%)	65 (28%)	63 (27%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	793/848 (94%)	366 (46%)	204 (26%)	223 (28%)	0 0

All (223) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	6	GLU
1	L	7	ARG
1	L	18	GLY
1	L	21	LEU
1	L	31	VAL
1	L	32	GLY
1	L	33	PHE
1	L	40	PHE
1	L	44	LEU
1	L	55	LEU
1	L	61	PRO
1	L	72	GLU
1	L	79	PRO
1	L	80	LEU
1	L	85	LEU
1	L	87	GLN
1	L	94	THR
1	L	108	CYS
1	L	109	ARG
1	L	113	ILE
1	L	128	TYR
1	L	129	LEU
1	L	147	PRO
1	L	150	ILE
1	L	171	PRO
1	L	172	ALA
1	L	186	ALA
1	L	213	ASP
1	L	223	SER
1	L	225	GLY
1	L	226	THR
1	L	237	SER
1	L	238	LEU
1	L	249	ILE
1	L	260	VAL
1	L	263	TRP
1	L	265	TRP

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Mol	Chain	Res	Type
2	M	8	SER
2	M	15	PRO
2	M	20	MET
2	M	22	GLU
2	M	24	VAL
2	M	25	ASN
2	M	29	ARG
2	M	34	PRO
2	M	38	LEU
2	M	39	LEU
2	M	46	GLN
2	M	47	LEU
2	M	82	PRO
2	M	99	PRO
2	M	103	LEU
2	M	105	PHE
2	M	106	ALA
2	M	114	LEU
2	M	122	MET
2	M	129	TRP
2	M	138	GLN
2	M	139	ALA
2	M	153	ALA
2	M	155	TRP
2	M	159	VAL
2	M	160	LEU
2	M	163	ILE
2	M	172	SER
2	M	209	LEU
2	M	213	ALA
2	M	228	ARG
2	M	244	ALA
2	M	245	ALA
2	M	246	GLU
2	M	258	PHE
2	M	262	MET
2	M	276	VAL
2	M	290	VAL
2	M	291	VAL
2	M	296	VAL
3	H	13	ALA
3	H	16	ALA

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Mol	Chain	Res	Type
3	H	21	TRP
3	H	28	ILE
3	H	31	LEU
3	H	32	GLN
3	H	38	GLU
3	H	41	PRO
3	H	49	PRO
3	H	51	ALA
3	H	53	GLN
3	H	80	SER
3	H	83	ARG
3	H	84	PRO
3	H	91	ALA
3	H	95	GLY
3	H	97	PRO
3	H	113	SER
3	H	116	ALA
3	H	130	LYS
3	H	176	ALA
3	H	200	SER
3	H	211	ASP
3	H	247	LYS
1	L	12	PRO
1	L	26	VAL
1	L	39	PHE
1	L	43	ALA
1	L	58	THR
1	L	59	TRP
1	L	71	LEU
1	L	84	GLY
1	L	140	GLY
1	L	145	ALA
1	L	148	TYR
1	L	153	HIS
1	L	161	GLY
1	L	174	MET
1	L	175	ILE
1	L	176	ALA
1	L	183	ASN
1	L	194	VAL
1	L	269	LEU
2	M	28	ASN

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Mol	Chain	Res	Type
2	M	32	VAL
2	M	53	GLY
2	M	59	SER
2	M	63	GLY
2	M	101	TYR
2	M	111	GLU
2	M	112	GLY
2	M	125	ALA
2	M	126	VAL
2	M	158	MET
2	M	191	LEU
2	M	195	ASN
2	M	223	ILE
2	M	257	GLY
2	M	295	TYR
3	H	23	PHE
3	H	42	LEU
3	H	55	PRO
3	H	92	VAL
3	H	115	VAL
3	H	118	ARG
3	H	123	LEU
3	H	125	GLY
3	H	128	HIS
3	H	129	ASN
3	H	136	ALA
3	H	144	ALA
3	H	157	ASP
3	H	158	LEU
3	H	172	PRO
3	H	186	GLY
3	H	196	VAL
3	H	209	SER
3	H	239	GLY
3	H	246	PRO
1	L	50	ALA
1	L	91	ILE
1	L	95	GLY
1	L	169	TYR
1	L	200	PRO
1	L	212	GLU
1	L	239	SER

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Mol	Chain	Res	Type
1	L	245	ALA
1	L	262	TRP
2	M	26	LEU
2	M	30	SER
2	M	96	PRO
2	M	118	ALA
2	M	152	SER
2	M	164	ARG
2	M	214	LEU
2	M	272	MET
2	M	279	THR
2	M	297	TRP
3	H	67	PRO
3	H	81	GLU
3	H	86	ALA
3	H	94	GLU
3	H	138	ALA
3	H	236	TYR
1	L	17	VAL
1	L	81	ALA
1	L	133	LEU
1	L	134	PHE
1	L	247	CYS
1	L	248	MET
2	M	149	ALA
2	M	288	GLY
3	H	46	ASP
3	H	58	LEU
3	H	59	PRO
3	H	112	ALA
3	H	156	CYS
3	H	207	ALA
3	H	212	LEU
3	H	241	LEU
1	L	49	ILE
1	L	78	ALA
1	L	165	GLY
1	L	193	LEU
1	L	243	PHE
2	M	13	ARG
2	M	84	VAL
2	M	93	SER

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Mol	Chain	Res	Type
3	H	78	PRO
1	L	47	ILE
1	L	105	VAL
1	L	136	PRO
2	M	58	LEU
2	M	222	THR
2	M	231	GLY
3	H	30	TYR
3	H	135	LYS
1	L	241	VAL
2	M	72	ILE
1	L	60	ASN
2	M	283	GLY
2	M	56	GLY
3	H	133	PRO
3	H	132	LYS
2	M	57	VAL
2	M	49	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	210/220 (96%)	124 (59%)	86 (41%)	0 0
2	M	232/240 (97%)	128 (55%)	104 (45%)	0 0
3	H	192/208 (92%)	92 (48%)	100 (52%)	0 0
All	All	634/668 (95%)	344 (54%)	290 (46%)	0 0

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	8	LYS
1	L	15	THR
1	L	16	LEU

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Mol	Chain	Res	Type
1	L	21	LEU
1	L	33	PHE
1	L	38	THR
1	L	44	LEU
1	L	46	ILE
1	L	47	ILE
1	L	49	ILE
1	L	51	TRP
1	L	52	SER
1	L	55	LEU
1	L	59	TRP
1	L	62	GLN
1	L	63	LEU
1	L	64	ILE
1	L	67	TYR
1	L	72	GLU
1	L	79	PRO
1	L	82	LYS
1	L	85	LEU
1	L	87	GLN
1	L	88	ILE
1	L	89	ILE
1	L	90	THR
1	L	91	ILE
1	L	98	VAL
1	L	99	SER
1	L	100	TRP
1	L	102	LEU
1	L	103	ARG
1	L	107	ILE
1	L	109	ARG
1	L	110	LYS
1	L	115	TYR
1	L	116	HIS
1	L	119	PHE
1	L	121	PHE
1	L	125	ILE
1	L	126	LEU
1	L	128	TYR
1	L	133	LEU
1	L	135	ARG
1	L	138	MET

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Mol	Chain	Res	Type
1	L	142	TRP
1	L	146	PHE
1	L	147	PRO
1	L	153	HIS
1	L	156	TRP
1	L	159	ASN
1	L	166	ASN
1	L	170	ASN
1	L	171	PRO
1	L	180	PHE
1	L	182	THR
1	L	183	ASN
1	L	185	LEU
1	L	187	LEU
1	L	202	LYS
1	L	205	GLU
1	L	207	ARG
1	L	208	THR
1	L	211	HIS
1	L	217	ARG
1	L	220	VAL
1	L	222	TYR
1	L	223	SER
1	L	227	LEU
1	L	229	ILE
1	L	232	LEU
1	L	235	LEU
1	L	242	PHE
1	L	243	PHE
1	L	247	CYS
1	L	248	MET
1	L	249	ILE
1	L	250	ILE
1	L	251	THR
1	L	257	ASP
1	L	261	ASP
1	L	265	TRP
1	L	267	VAL
1	L	268	LYS
1	L	269	LEU
2	M	7	PHE
2	M	11	GLN

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Mol	Chain	Res	Type
2	M	13	ARG
2	M	18	LEU
2	M	20	MET
2	M	22	GLU
2	M	23	ASP
2	M	25	ASN
2	M	26	LEU
2	M	29	ARG
2	M	30	SER
2	M	32	VAL
2	M	34	PRO
2	M	35	PHE
2	M	37	THR
2	M	39	LEU
2	M	44	ASN
2	M	47	LEU
2	M	50	ILE
2	M	51	TYR
2	M	52	LEU
2	M	55	LEU
2	M	57	VAL
2	M	58	LEU
2	M	59	SER
2	M	60	LEU
2	M	65	MET
2	M	67	PHE
2	M	70	ILE
2	M	72	ILE
2	M	74	PHE
2	M	76	TYR
2	M	77	GLN
2	M	82	PRO
2	M	87	ARG
2	M	93	SER
2	M	95	GLU
2	M	100	GLU
2	M	101	TYR
2	M	103	LEU
2	M	104	SER
2	M	105	PHE
2	M	109	LEU
2	M	110	LYS

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Mol	Chain	Res	Type
2	M	114	LEU
2	M	119	SER
2	M	120	PHE
2	M	121	PHE
2	M	122	MET
2	M	126	VAL
2	M	133	THR
2	M	134	TYR
2	M	135	LEU
2	M	136	ARG
2	M	144	LYS
2	M	145	HIS
2	M	148	TRP
2	M	152	SER
2	M	155	TRP
2	M	160	LEU
2	M	164	ARG
2	M	165	PRO
2	M	166	ILE
2	M	168	MET
2	M	172	SER
2	M	179	ILE
2	M	182	HIS
2	M	185	TRP
2	M	187	ASN
2	M	190	SER
2	M	191	LEU
2	M	205	SER
2	M	209	LEU
2	M	214	LEU
2	M	216	PHE
2	M	218	MET
2	M	227	SER
2	M	228	ARG
2	M	229	PHE
2	M	232	GLU
2	M	233	ARG
2	M	235	LEU
2	M	236	GLU
2	M	238	ILE
2	M	240	ASP
2	M	241	ARG

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Mol	Chain	Res	Type
2	M	243	THR
2	M	250	LEU
2	M	253	ARG
2	M	258	PHE
2	M	259	ASN
2	M	261	THR
2	M	263	GLU
2	M	267	ARG
2	M	268	TRP
2	M	270	ILE
2	M	271	TRP
2	M	274	VAL
2	M	275	LEU
2	M	277	THR
2	M	278	LEU
2	M	279	THR
2	M	299	GLN
2	M	300	ASN
3	H	12	LEU
3	H	14	SER
3	H	15	LEU
3	H	17	ILE
3	H	18	TYR
3	H	20	PHE
3	H	23	PHE
3	H	24	LEU
3	H	27	LEU
3	H	29	TYR
3	H	30	TYR
3	H	33	THR
3	H	34	GLU
3	H	35	ASN
3	H	36	MET
3	H	37	ARG
3	H	38	GLU
3	H	40	TYR
3	H	42	LEU
3	H	44	ASN
3	H	46	ASP
3	H	53	GLN
3	H	56	PHE
3	H	60	LYS

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Mol	Chain	Res	Type
3	H	62	LYS
3	H	63	THR
3	H	64	PHE
3	H	65	ILE
3	H	66	LEU
3	H	68	HIS
3	H	74	THR
3	H	79	GLU
3	H	82	ASP
3	H	83	ARG
3	H	85	ILE
3	H	92	VAL
3	H	93	SER
3	H	94	GLU
3	H	105	MET
3	H	106	LYS
3	H	107	ASP
3	H	109	VAL
3	H	113	SER
3	H	115	VAL
3	H	117	ARG
3	H	118	ARG
3	H	119	ASP
3	H	123	LEU
3	H	124	ASP
3	H	126	HIS
3	H	128	HIS
3	H	129	ASN
3	H	131	ILE
3	H	134	MET
3	H	135	LYS
3	H	141	HIS
3	H	151	LEU
3	H	156	CYS
3	H	158	LEU
3	H	159	GLU
3	H	160	ILE
3	H	163	LYS
3	H	166	ASP
3	H	171	ILE
3	H	174	GLN
3	H	178	PHE

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Mol	Chain	Res	Type
3	H	179	LEU
3	H	182	GLU
3	H	183	LEU
3	H	184	LYS
3	H	185	ASP
3	H	188	THR
3	H	189	ARG
3	H	194	GLN
3	H	195	MET
3	H	196	VAL
3	H	197	LYS
3	H	199	GLN
3	H	204	HIS
3	H	205	VAL
3	H	209	SER
3	H	210	SER
3	H	211	ASP
3	H	212	LEU
3	H	213	PHE
3	H	219	ILE
3	H	220	LYS
3	H	221	SER
3	H	223	THR
3	H	228	LEU
3	H	229	GLU
3	H	231	ASP
3	H	232	LYS
3	H	234	CYS
3	H	237	VAL
3	H	241	LEU
3	H	242	MET
3	H	243	TYR
3	H	247	LYS
3	H	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
1	L	62	GLN
1	L	116	HIS
1	L	153	HIS

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Mol	Chain	Res	Type
1	L	168	HIS
1	L	211	HIS
2	M	9	GLN
2	M	25	ASN
2	M	28	ASN
2	M	44	ASN
2	M	46	GLN
2	M	77	GLN
2	M	145	HIS
2	M	187	ASN
2	M	299	GLN
2	M	301	HIS
3	H	35	ASN
3	H	98	HIS
3	H	199	GLN
3	H	204	HIS
3	H	206	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BOG	M	308	-	20,20,20	0.66	0	25,25,25	1.40	3 (12%)
6	U10	M	313	-	51,51,63	0.96	1 (1%)	61,64,79	2.00	20 (32%)
4	BCL	M	311	-	49,59,74	3.08	14 (28%)	60,97,115	3.21	26 (43%)
4	BCL	L	282	2	49,59,74	1.88	9 (18%)	60,97,115	3.00	23 (38%)
4	BCL	M	310	2	64,74,74	1.87	11 (17%)	78,115,115	2.91	25 (32%)
4	BCL	L	283	1	64,74,74	1.82	10 (15%)	78,115,115	2.84	29 (37%)
6	U10	L	285	-	41,41,63	1.01	0	49,52,79	1.87	13 (26%)
5	BPH	M	312	2	51,70,70	1.75	6 (11%)	52,101,101	2.62	17 (32%)
5	BPH	L	284	-	51,70,70	1.32	4 (7%)	52,101,101	2.20	15 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BOG	M	308	-	1/1/5/5	8/11/31/31	0/1/1/1
5	BPH	L	284	-	-	12/37/105/105	0/5/6/6
6	U10	M	313	-	-	18/49/73/87	0/1/1/1
4	BCL	L	282	2	-	10/19/119/137	-
4	BCL	M	310	2	-	20/37/137/137	-
4	BCL	L	283	1	-	13/37/137/137	-
6	U10	L	285	-	-	17/37/61/87	0/1/1/1
5	BPH	M	312	2	-	18/37/105/105	0/5/6/6
4	BCL	M	311	-	-	5/19/119/137	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	311	BCL	MG-ND	16.39	2.38	2.05
5	M	312	BPH	C6-C7	6.21	1.78	1.52
4	L	282	BCL	O1D-CGD	5.71	1.35	1.21
5	M	312	BPH	C11-C10	5.60	1.76	1.52
4	M	310	BCL	MG-ND	5.58	2.16	2.05
4	M	310	BCL	O1D-CGD	5.35	1.34	1.21
4	M	310	BCL	C4B-NB	5.32	1.40	1.35
4	L	283	BCL	MG-ND	5.30	2.16	2.05
4	L	283	BCL	O1D-CGD	5.28	1.34	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	311	BCL	O1D-CGD	5.07	1.33	1.21
4	L	282	BCL	C4B-NB	5.02	1.39	1.35
5	M	312	BPH	O1D-CGD	5.01	1.33	1.21
4	M	310	BCL	C1B-NB	4.98	1.39	1.35
4	L	282	BCL	C1B-NB	4.90	1.39	1.35
5	L	284	BPH	O2D-CGD	-4.90	1.21	1.33
4	L	283	BCL	MG-NC	4.84	2.17	2.06
5	M	312	BPH	O2D-CGD	-4.83	1.21	1.33
4	M	311	BCL	CAA-C2A	4.82	1.63	1.54
4	M	311	BCL	C4B-NB	4.80	1.39	1.35
4	L	283	BCL	C1B-NB	4.77	1.39	1.35
4	L	283	BCL	C4B-NB	4.41	1.39	1.35
5	L	284	BPH	O1D-CGD	4.27	1.31	1.21
4	L	283	BCL	MG-NA	4.20	2.16	2.06
4	M	310	BCL	MG-NA	4.17	2.16	2.06
4	M	310	BCL	O2D-CGD	-4.14	1.23	1.33
4	L	282	BCL	C4D-ND	4.09	1.43	1.37
4	M	310	BCL	MG-NC	4.02	2.15	2.06
4	M	310	BCL	C4D-ND	3.87	1.43	1.37
4	M	311	BCL	CMA-C3A	-3.79	1.45	1.53
4	M	311	BCL	C1B-NB	3.74	1.38	1.35
5	L	284	BPH	C3B-C2B	-3.67	1.32	1.39
4	M	311	BCL	MG-NC	3.47	2.14	2.06
4	L	282	BCL	O2D-CGD	-3.42	1.24	1.33
4	L	282	BCL	CAC-C3C	-3.39	1.47	1.54
4	L	283	BCL	O2D-CGD	-3.35	1.25	1.33
4	L	282	BCL	MG-ND	3.31	2.12	2.05
4	L	283	BCL	C4D-ND	3.24	1.42	1.37
4	M	311	BCL	C1A-CHA	3.22	1.56	1.43
4	M	311	BCL	CAC-C3C	-3.00	1.48	1.54
4	L	283	BCL	CAC-C3C	-2.98	1.48	1.54
4	M	311	BCL	O2D-CGD	-2.89	1.26	1.33
5	M	312	BPH	CAC-C3C	-2.88	1.47	1.53
4	M	311	BCL	C4D-ND	2.86	1.41	1.37
4	M	311	BCL	MG-NA	2.80	2.12	2.06
4	M	311	BCL	O2D-CED	2.71	1.51	1.45
4	M	311	BCL	C4D-CHA	2.64	1.47	1.38
5	M	312	BPH	C3B-C2B	-2.58	1.34	1.39
4	M	310	BCL	CAC-C3C	-2.40	1.49	1.54
4	L	283	BCL	O2A-C1	2.39	1.52	1.46
6	M	313	U10	C16-C14	2.34	1.56	1.51
4	L	282	BCL	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	310	BCL	C1-C2	2.06	1.55	1.49
4	M	310	BCL	O2D-CED	2.04	1.50	1.45
4	L	282	BCL	CAA-C2A	2.03	1.57	1.54
5	L	284	BPH	C1-C2	2.02	1.55	1.49

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	310	BCL	C4D-C3D-CAD	-13.35	92.36	108.10
4	M	311	BCL	C4D-C3D-CAD	-12.94	92.84	108.10
4	L	282	BCL	C4D-C3D-CAD	-12.45	93.42	108.10
4	L	283	BCL	C4D-C3D-CAD	-12.27	93.63	108.10
4	M	310	BCL	C3D-C4D-CHA	7.57	130.03	112.72
5	M	312	BPH	C7-C6-C5	7.37	133.38	113.36
4	L	282	BCL	C3D-C4D-CHA	6.99	128.71	112.72
4	M	311	BCL	C1C-NC-C4C	6.90	109.81	106.71
4	M	310	BCL	C1C-NC-C4C	6.89	109.80	106.71
4	L	283	BCL	C3D-C4D-CHA	6.88	128.47	112.72
5	M	312	BPH	C11-C10-C8	6.75	137.75	115.92
5	L	284	BPH	O1D-CGD-CBD	-6.51	113.89	124.74
4	M	311	BCL	C3D-C4D-CHA	6.45	127.49	112.72
5	M	312	BPH	O1D-CGD-CBD	-6.44	114.02	124.74
4	M	310	BCL	C4D-CHA-C1A	6.42	129.07	121.25
4	L	283	BCL	CMB-C2B-C1B	-6.31	118.76	128.46
4	M	311	BCL	C1D-ND-C4D	6.30	110.81	106.33
4	L	283	BCL	C4D-CHA-C1A	6.26	128.87	121.25
5	M	312	BPH	O2D-CGD-CBD	6.17	118.81	111.00
4	L	282	BCL	C4D-CHA-C1A	6.08	128.65	121.25
4	L	283	BCL	C4-C3-C5	6.03	125.41	115.27
4	M	311	BCL	CMB-C2B-C1B	-5.89	119.41	128.46
4	M	310	BCL	C4A-NA-C1A	5.73	109.28	106.71
4	M	310	BCL	CMB-C2B-C1B	-5.59	119.87	128.46
4	L	283	BCL	C1C-NC-C4C	5.45	109.16	106.71
5	L	284	BPH	C3D-CAD-CBD	5.43	114.75	107.61
6	L	285	U10	C12-C13-C14	-5.39	114.68	127.66
5	L	284	BPH	CMD-C2D-C3D	5.37	134.72	124.68
4	L	282	BCL	CMB-C2B-C1B	-5.31	120.30	128.46
5	M	312	BPH	CMD-C2D-C3D	5.19	134.39	124.68
4	M	311	BCL	C4A-NA-C1A	5.18	109.04	106.71
4	M	310	BCL	O2D-CGD-CBD	5.18	120.47	111.27
4	L	282	BCL	C1-C2-C3	-5.17	118.38	126.75
5	M	312	BPH	C3D-CAD-CBD	5.06	114.26	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	283	BCL	C4A-NA-C1A	4.87	108.90	106.71
4	M	311	BCL	CMB-C2B-C3B	4.86	133.76	124.68
4	M	310	BCL	C1D-ND-C4D	4.76	109.72	106.33
6	M	313	U10	C7-C8-C9	-4.72	118.93	126.79
4	M	311	BCL	CAA-CBA-CGA	4.68	126.94	113.25
4	L	282	BCL	O2D-CGD-CBD	4.66	119.55	111.27
6	L	285	U10	C27-C28-C29	-4.58	116.64	127.66
4	L	283	BCL	C1D-ND-C4D	4.55	109.57	106.33
5	M	312	BPH	CMB-C2B-C3B	4.45	133.01	124.68
5	L	284	BPH	O2D-CGD-O1D	4.42	132.49	123.84
4	L	283	BCL	CMB-C2B-C3B	4.39	132.90	124.68
5	M	312	BPH	C6-C7-C8	-4.39	101.73	115.92
6	M	313	U10	C17-C18-C19	-4.26	117.40	127.66
4	L	282	BCL	OBD-CAD-C3D	-4.26	118.27	128.52
4	L	282	BCL	C1C-NC-C4C	4.21	108.60	106.71
4	L	282	BCL	C1D-ND-C4D	4.16	109.29	106.33
4	L	282	BCL	CMD-C2D-C1D	-4.15	117.40	124.71
4	M	310	BCL	CMB-C2B-C3B	4.14	132.41	124.68
4	L	282	BCL	C4A-NA-C1A	4.07	108.54	106.71
4	M	311	BCL	CMD-C2D-C1D	-4.07	117.54	124.71
4	M	310	BCL	CMD-C2D-C1D	-4.05	117.58	124.71
5	L	284	BPH	CMB-C2B-C3B	4.00	132.16	124.68
6	M	313	U10	C30-C29-C31	4.00	121.99	115.27
4	M	310	BCL	C4-C3-C5	3.99	121.98	115.27
4	M	311	BCL	CAA-C2A-C3A	-3.95	101.95	112.78
6	M	313	U10	C22-C23-C24	-3.95	118.14	127.66
4	M	310	BCL	O1D-CGD-CBD	-3.95	116.40	124.48
4	M	310	BCL	CHA-C4D-ND	-3.79	124.56	132.50
4	L	283	BCL	C1-C2-C3	-3.79	119.49	126.04
6	M	313	U10	C1M-C1-C6	-3.79	118.22	124.40
4	L	282	BCL	CMB-C2B-C3B	3.78	131.74	124.68
4	M	311	BCL	OBB-CAB-C3B	3.76	126.67	119.99
4	L	283	BCL	CMD-C2D-C1D	-3.75	118.11	124.71
6	M	313	U10	C32-C33-C34	-3.72	118.70	127.66
4	M	311	BCL	C2D-C1D-ND	-3.71	107.37	110.10
4	M	310	BCL	CAD-C3D-C2D	3.59	158.12	140.80
5	L	284	BPH	CAC-C3C-C2C	-3.58	105.32	114.26
4	M	311	BCL	CAD-C3D-C2D	3.55	157.94	140.80
6	M	313	U10	C17-C16-C14	-3.53	101.38	112.98
4	M	311	BCL	C3D-C4D-ND	-3.49	104.58	110.24
4	M	311	BCL	O2A-CGA-O1A	-3.48	114.80	123.59
5	M	312	BPH	CMC-C2C-C1C	-3.47	106.79	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	313	U10	C16-C14-C13	-3.44	114.16	121.12
4	M	310	BCL	OBD-CAD-C3D	-3.38	120.39	128.52
4	L	283	BCL	CAD-C3D-C2D	3.37	157.06	140.80
4	L	283	BCL	CHA-C4D-ND	-3.35	125.49	132.50
4	M	311	BCL	CBB-CAB-C3B	-3.33	110.44	120.34
4	L	282	BCL	CHA-C4D-ND	-3.32	125.55	132.50
5	L	284	BPH	C16-C15-C13	-3.32	105.20	115.92
4	L	283	BCL	C16-C15-C13	-3.29	105.28	115.92
4	M	310	BCL	C2D-C1D-ND	-3.29	107.68	110.10
5	L	284	BPH	C1-C2-C3	-3.27	120.39	126.04
6	M	313	U10	C25-C24-C26	3.26	120.75	115.27
4	L	282	BCL	CAD-C3D-C2D	3.24	156.45	140.80
4	L	283	BCL	C2D-C1D-ND	-3.24	107.72	110.10
4	M	311	BCL	OBD-CAD-C3D	-3.17	120.89	128.52
6	L	285	U10	C10-C9-C11	3.15	120.58	115.27
4	M	310	BCL	CAC-C3C-C2C	-3.12	106.47	114.26
5	L	284	BPH	OBB-CAB-CBB	3.12	127.18	120.17
4	L	283	BCL	C11-C12-C13	-3.10	105.89	115.92
6	M	313	U10	C27-C28-C29	-3.09	120.23	127.66
6	L	285	U10	C20-C19-C21	3.08	120.45	115.27
4	M	310	BCL	C3D-C4D-ND	-3.06	105.29	110.24
4	M	311	BCL	CMD-C2D-C3D	3.05	134.64	127.61
4	L	282	BCL	C2D-C1D-ND	-3.03	107.87	110.10
6	L	285	U10	C30-C29-C31	3.01	120.34	115.27
4	M	310	BCL	CMD-C2D-C3D	2.98	134.47	127.61
4	M	311	BCL	CGD-CBD-CAD	-2.98	101.08	110.73
4	L	283	BCL	C5-C3-C2	-2.97	115.11	121.12
4	L	282	BCL	CMD-C2D-C3D	2.96	134.41	127.61
4	L	282	BCL	C3D-C4D-ND	-2.95	105.46	110.24
7	M	308	BOG	C1'-O1-C1	2.94	118.72	113.84
4	M	310	BCL	CMC-C2C-C1C	-2.94	103.86	111.77
5	L	284	BPH	C1-O2A-CGA	2.94	124.16	116.44
7	M	308	BOG	O5-C1-C2	-2.94	104.14	110.35
7	M	308	BOG	O5-C5-C6	2.92	113.70	106.44
5	M	312	BPH	CED-O2D-CGD	2.89	122.46	115.94
6	M	313	U10	C10-C9-C11	2.85	120.07	115.27
4	L	283	BCL	CMD-C2D-C3D	2.80	134.05	127.61
4	M	311	BCL	C1-C2-C3	-2.79	122.24	126.75
4	L	283	BCL	C1-O2A-CGA	-2.79	109.14	116.44
4	L	283	BCL	C3D-C4D-ND	-2.78	105.74	110.24
4	L	283	BCL	CMA-C3A-C2A	-2.77	102.66	113.83
4	L	283	BCL	CAA-CBA-CGA	-2.75	105.22	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	313	U10	C12-C13-C14	-2.74	121.07	127.66
6	L	285	U10	C11-C12-C13	-2.71	102.98	111.88
6	L	285	U10	C1M-C1-C6	-2.71	119.98	124.40
5	L	284	BPH	CED-O2D-CGD	2.71	122.06	115.94
6	L	285	U10	C25-C24-C26	2.70	119.81	115.27
6	M	313	U10	C20-C19-C21	2.70	119.81	115.27
5	L	284	BPH	CMC-C2C-C1C	-2.70	108.47	114.38
4	M	311	BCL	O2D-CGD-CBD	2.69	116.04	111.27
6	L	285	U10	C7-C8-C9	-2.67	122.34	126.79
6	L	285	U10	C17-C18-C19	-2.60	121.39	127.66
5	M	312	BPH	C1-O2A-CGA	-2.59	109.64	116.44
4	M	311	BCL	CMA-C3A-C4A	2.58	118.71	111.77
4	M	311	BCL	CHB-C4A-NA	2.53	128.01	124.51
5	M	312	BPH	OBB-CAB-CBB	2.50	125.80	120.17
4	L	283	BCL	C4B-C3B-CAB	-2.50	122.30	127.13
4	L	283	BCL	C11-C10-C8	-2.48	107.91	115.92
4	L	282	BCL	CAC-C3C-C2C	-2.47	108.08	114.26
4	L	282	BCL	C5-C3-C4	2.47	120.05	114.60
6	M	313	U10	C35-C34-C36	2.46	119.41	115.27
4	M	310	BCL	C1-C2-C3	-2.46	121.79	126.04
6	M	313	U10	C27-C26-C24	-2.45	104.93	112.98
4	L	283	BCL	OBD-CAD-C3D	-2.43	122.68	128.52
4	M	310	BCL	C3A-C2A-C1A	2.42	104.97	101.34
4	M	310	BCL	C11-C12-C13	-2.41	108.14	115.92
5	L	284	BPH	CMA-C3A-C4A	-2.39	109.14	114.38
4	M	311	BCL	CHA-C4D-ND	-2.34	127.59	132.50
4	L	282	BCL	CMA-C3A-C2A	-2.33	104.41	113.83
4	L	282	BCL	O1D-CGD-CBD	-2.33	119.71	124.48
6	L	285	U10	C15-C14-C16	2.30	119.14	115.27
6	L	285	U10	C17-C16-C14	-2.29	105.44	112.98
6	M	313	U10	C35-C34-C33	-2.28	117.83	123.68
6	M	313	U10	C31-C29-C28	-2.25	116.56	121.12
4	L	283	BCL	O2A-CGA-CBA	2.20	118.82	111.91
5	M	312	BPH	CAA-C2A-C3A	-2.20	106.75	112.78
4	L	282	BCL	CAC-C3C-C4C	2.20	117.46	112.58
5	M	312	BPH	O2A-C1-C2	2.19	114.39	108.64
4	M	310	BCL	C4B-C3B-CAB	-2.19	122.91	127.13
4	M	311	BCL	O1D-CGD-CBD	-2.14	120.10	124.48
6	M	313	U10	C40-C39-C41	2.14	118.87	115.27
4	L	283	BCL	C1B-CHB-C4A	-2.13	125.89	130.12
6	M	313	U10	C26-C24-C23	-2.13	116.81	121.12
4	L	283	BCL	C4-C3-C2	-2.12	118.24	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	284	BPH	CBC-CAC-C3C	-2.08	109.58	113.77
4	L	283	BCL	O2D-CGD-CBD	2.06	114.93	111.27
6	M	313	U10	C37-C38-C39	-2.06	122.70	127.66
5	M	312	BPH	O2A-CGA-O1A	-2.04	118.44	123.59
5	M	312	BPH	CMA-C3A-C2A	-2.04	105.79	113.99
4	M	311	BCL	O2D-CGD-O1D	-2.03	119.86	123.84
4	L	282	BCL	CGD-CBD-CAD	2.03	117.32	110.73
6	L	285	U10	C20-C19-C18	-2.02	118.49	123.68
5	L	284	BPH	C14-C13-C15	-2.02	103.97	111.29
5	M	312	BPH	C16-C15-C13	-2.01	109.42	115.92
4	M	310	BCL	C4-C3-C2	-2.00	118.55	123.68

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	M	308	BOG	C1

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	282	BCL	C3A-C2A-CAA-CBA
4	L	282	BCL	C2C-C3C-CAC-CBC
4	L	282	BCL	C4C-C3C-CAC-CBC
4	L	282	BCL	CHA-CBD-CGD-O1D
4	L	283	BCL	C2C-C3C-CAC-CBC
4	L	283	BCL	C4C-C3C-CAC-CBC
4	M	310	BCL	C1A-C2A-CAA-CBA
4	M	310	BCL	C3A-C2A-CAA-CBA
4	M	310	BCL	C2A-CAA-CBA-CGA
4	M	310	BCL	C2C-C3C-CAC-CBC
4	M	310	BCL	C4C-C3C-CAC-CBC
4	M	310	BCL	CHA-CBD-CGD-O1D
4	M	310	BCL	CAD-CBD-CGD-O1D
4	M	310	BCL	CAD-CBD-CGD-O2D
4	M	311	BCL	CHA-CBD-CGD-O1D
4	M	311	BCL	CBD-CGD-O2D-CED
5	L	284	BPH	C2C-C3C-CAC-CBC
5	L	284	BPH	C3A-C2A-CAA-CBA
5	L	284	BPH	C1A-C2A-CAA-CBA
5	M	312	BPH	CBD-CGD-O2D-CED
5	M	312	BPH	C3A-C2A-CAA-CBA
5	M	312	BPH	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	M	312	BPH	C4-C3-C5-C6
6	L	285	U10	C1-C6-C7-C8
6	L	285	U10	C5-C6-C7-C8
6	L	285	U10	C11-C12-C13-C14
6	L	285	U10	C14-C16-C17-C18
6	L	285	U10	C19-C21-C22-C23
6	L	285	U10	C29-C31-C32-C33
6	M	313	U10	C3-C4-O4-C4M
6	M	313	U10	C21-C22-C23-C24
5	M	312	BPH	O1D-CGD-O2D-CED
4	M	311	BCL	O1D-CGD-O2D-CED
4	M	310	BCL	O1A-CGA-O2A-C1
5	M	312	BPH	C3-C5-C6-C7
4	M	310	BCL	CBA-CGA-O2A-C1
5	M	312	BPH	C2-C3-C5-C6
5	M	312	BPH	CBA-CGA-O2A-C1
7	M	308	BOG	O5-C5-C6-O6
5	M	312	BPH	O1A-CGA-O2A-C1
5	L	284	BPH	CBD-CGD-O2D-CED
4	M	310	BCL	C4-C3-C5-C6
6	L	285	U10	C25-C24-C26-C27
4	M	310	BCL	C2-C3-C5-C6
6	L	285	U10	C23-C24-C26-C27
7	M	308	BOG	C2'-C3'-C4'-C5'
7	M	308	BOG	O5-C1-O1-C1'
6	L	285	U10	C9-C11-C12-C13
6	M	313	U10	C24-C26-C27-C28
6	M	313	U10	C34-C36-C37-C38
7	M	308	BOG	C2-C1-O1-C1'
6	L	285	U10	C30-C29-C31-C32
4	L	283	BCL	C6-C7-C8-C9
5	L	284	BPH	C14-C13-C15-C16
4	M	310	BCL	C13-C15-C16-C17
6	M	313	U10	C41-C42-C43-C44
7	M	308	BOG	C4-C5-C6-O6
5	L	284	BPH	C3-C5-C6-C7
5	M	312	BPH	C15-C16-C17-C18
6	L	285	U10	C24-C26-C27-C28
6	M	313	U10	C14-C16-C17-C18
6	M	313	U10	C39-C41-C42-C43
4	M	310	BCL	C14-C13-C15-C16
6	L	285	U10	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	M	313	U10	C36-C37-C38-C39
5	M	312	BPH	C16-C17-C18-C19
4	L	283	BCL	C3A-C2A-CAA-CBA
4	M	310	BCL	C6-C7-C8-C10
4	M	310	BCL	C12-C13-C15-C16
5	L	284	BPH	C11-C10-C8-C7
5	M	312	BPH	C16-C17-C18-C20
4	L	283	BCL	C2-C3-C5-C6
6	L	285	U10	C28-C29-C31-C32
6	M	313	U10	C18-C19-C21-C22
4	M	310	BCL	C6-C7-C8-C9
5	L	284	BPH	C11-C10-C8-C9
4	L	282	BCL	C1A-C2A-CAA-CBA
4	L	283	BCL	C1A-C2A-CAA-CBA
4	M	311	BCL	C1A-C2A-CAA-CBA
7	M	308	BOG	O1-C1'-C2'-C3'
5	L	284	BPH	C10-C11-C12-C13
6	M	313	U10	C20-C19-C21-C22
4	M	311	BCL	C1-C2-C3-C4
4	L	283	BCL	C6-C7-C8-C10
5	L	284	BPH	C8-C10-C11-C12
4	L	283	BCL	C2A-CAA-CBA-CGA
7	M	308	BOG	C4'-C5'-C6'-C7'
4	L	283	BCL	C16-C17-C18-C19
5	L	284	BPH	C12-C13-C15-C16
4	L	283	BCL	CBA-CGA-O2A-C1
5	M	312	BPH	C8-C10-C11-C12
6	M	313	U10	C5-C4-O4-C4M
4	L	282	BCL	CHA-CBD-CGD-O2D
6	M	313	U10	C1-C6-C7-C8
4	L	283	BCL	C13-C15-C16-C17
4	L	283	BCL	O1D-CGD-O2D-CED
4	L	283	BCL	C16-C17-C18-C20
5	L	284	BPH	CHA-CBD-CGD-O1D
5	M	312	BPH	CHA-CBD-CGD-O2D
4	L	282	BCL	O1D-CGD-O2D-CED
6	M	313	U10	C2-C3-O3-C3M
6	L	285	U10	C31-C32-C33-C34
4	L	282	BCL	CBA-CGA-O2A-C1
5	M	312	BPH	C11-C10-C8-C9
6	M	313	U10	C35-C34-C36-C37
6	M	313	U10	C40-C39-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	M	310	BCL	C11-C10-C8-C7
4	L	282	BCL	C2A-CAA-CBA-CGA
4	L	282	BCL	C2-C1-O2A-CGA
6	M	313	U10	C13-C14-C16-C17
4	M	310	BCL	C11-C10-C8-C9
7	M	308	BOG	C3'-C4'-C5'-C6'
4	M	310	BCL	CHA-CBD-CGD-O2D
6	L	285	U10	C13-C14-C16-C17
6	M	313	U10	C31-C32-C33-C34
6	L	285	U10	C16-C17-C18-C19
5	M	312	BPH	CAA-CBA-CGA-O1A
6	M	313	U10	C26-C27-C28-C29
5	M	312	BPH	C6-C7-C8-C10
5	M	312	BPH	CAA-CBA-CGA-O2A
6	L	285	U10	C4-C3-O3-C3M

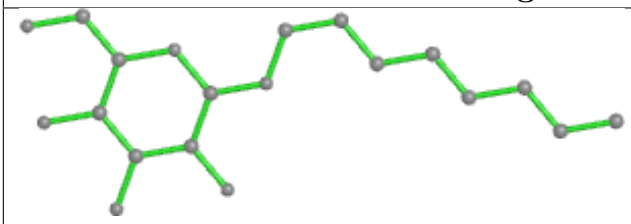
There are no ring outliers.

9 monomers are involved in 327 short contacts:

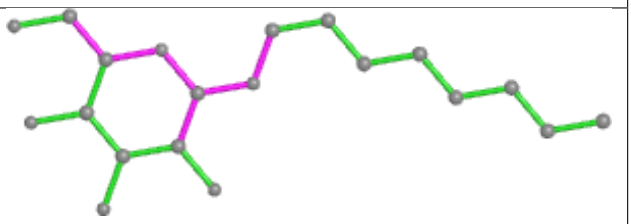
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	308	BOG	7	0
6	M	313	U10	43	0
4	M	311	BCL	25	0
4	L	282	BCL	19	0
4	M	310	BCL	68	0
4	L	283	BCL	100	0
6	L	285	U10	31	0
5	M	312	BPH	47	0
5	L	284	BPH	44	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

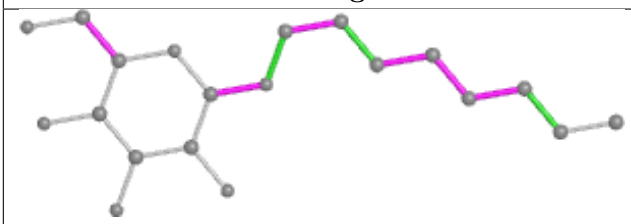
Ligand BOG M 308



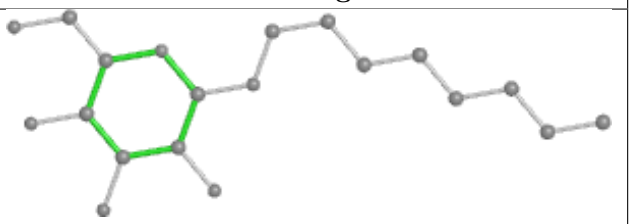
Bond lengths



Bond angles

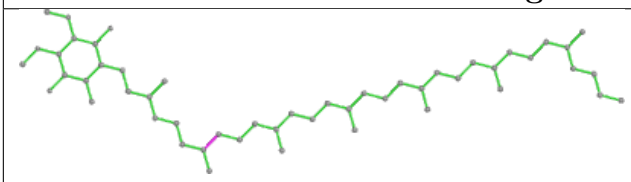


Torsions

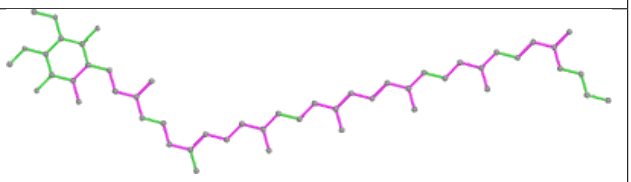


Rings

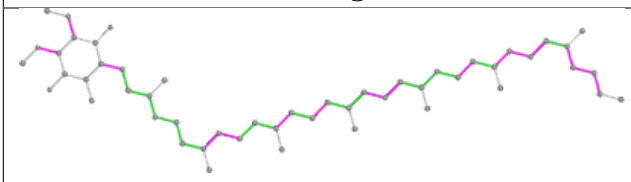
Ligand U10 M 313



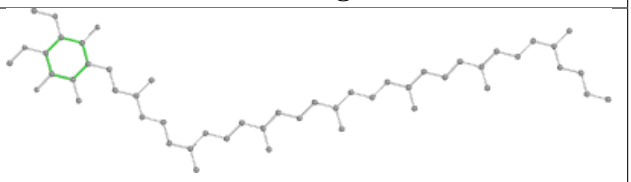
Bond lengths



Bond angles

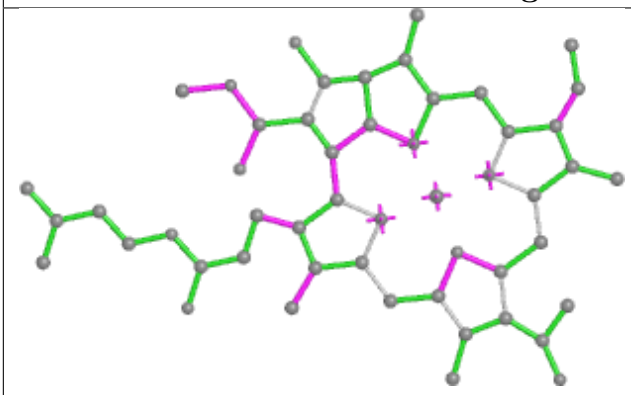


Torsions

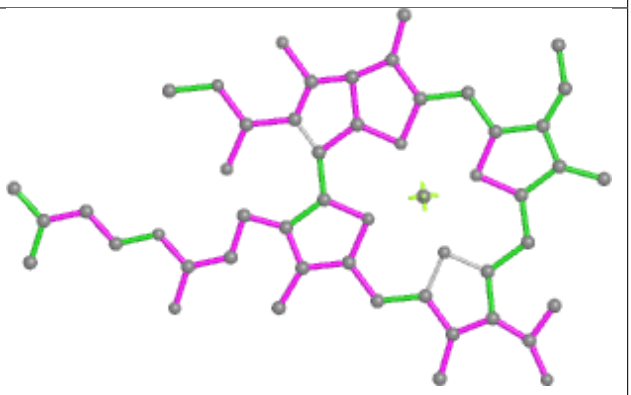


Rings

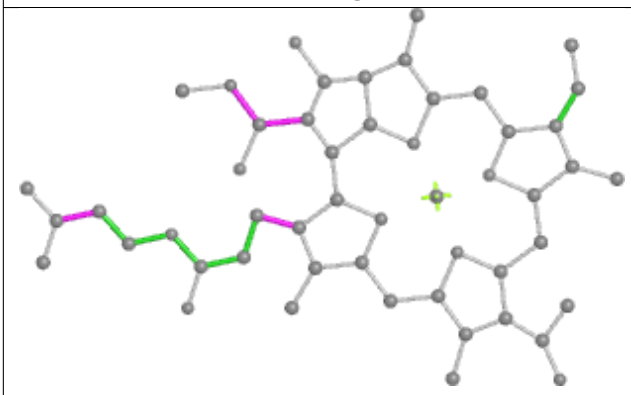
Ligand BCL M 311



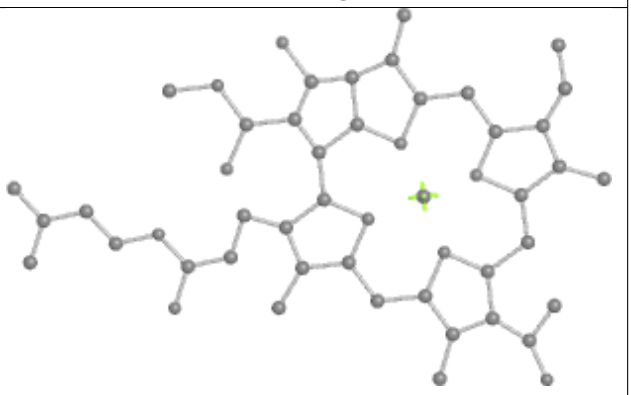
Bond lengths



Bond angles

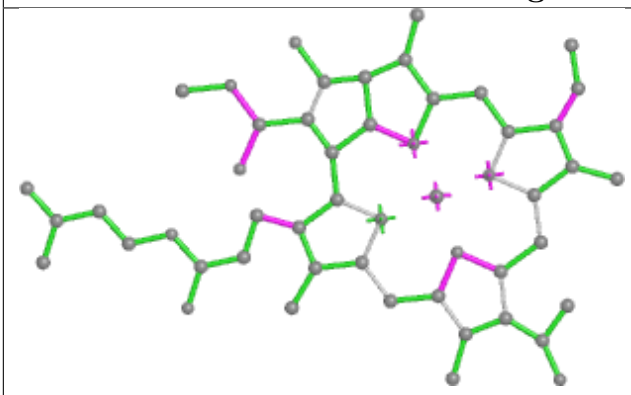


Torsions

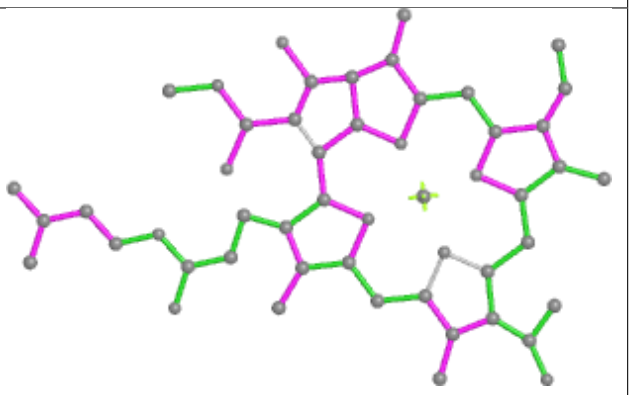


Rings

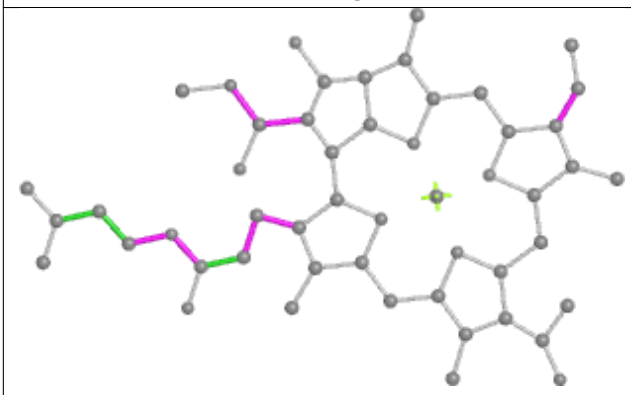
Ligand BCL L 282



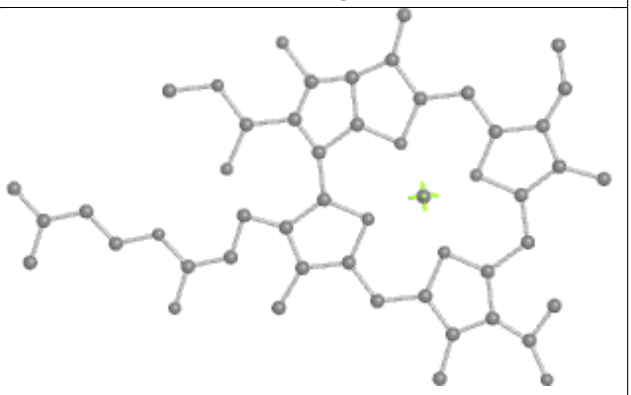
Bond lengths



Bond angles

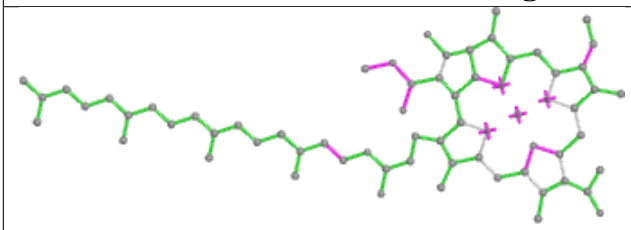


Torsions

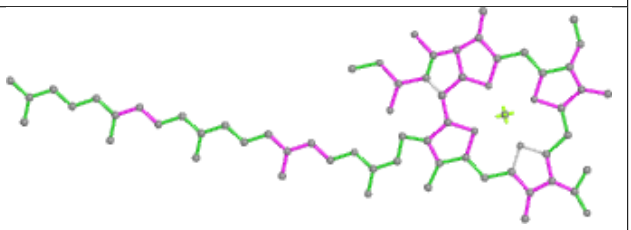


Rings

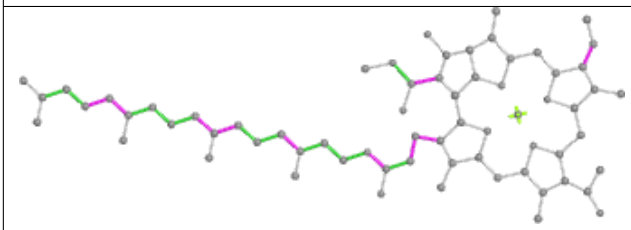
Ligand BCL M 310



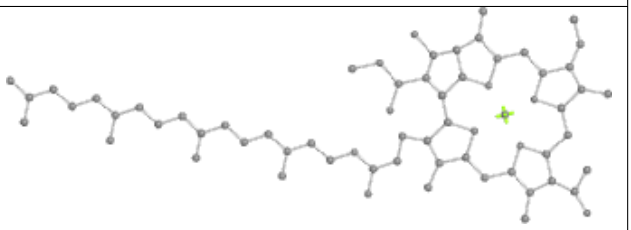
Bond lengths



Bond angles

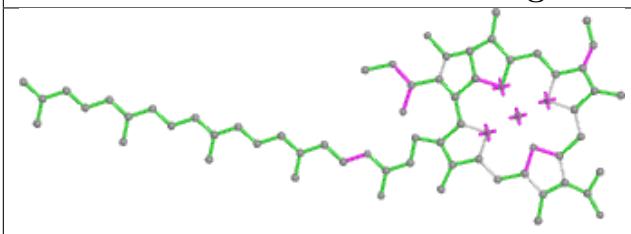


Torsions

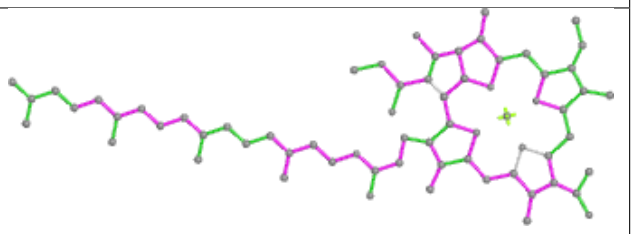


Rings

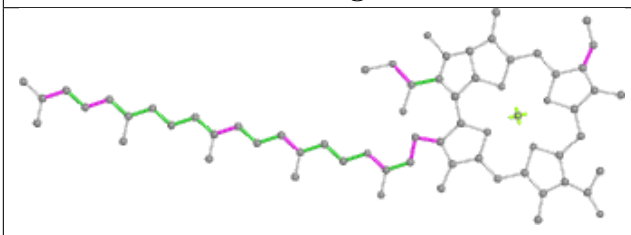
Ligand BCL L 283



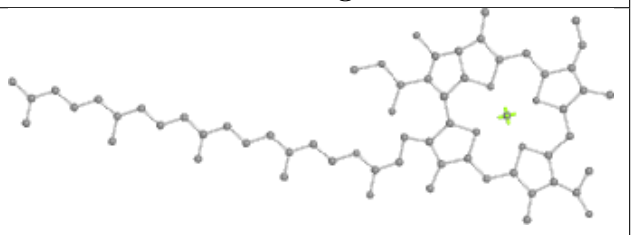
Bond lengths



Bond angles

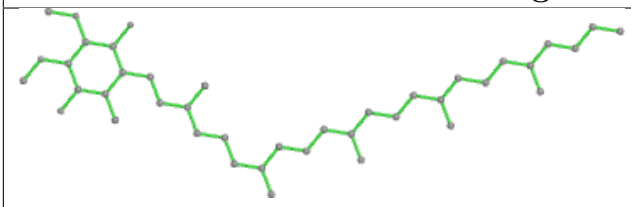


Torsions

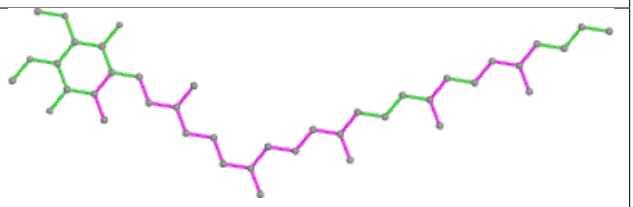


Rings

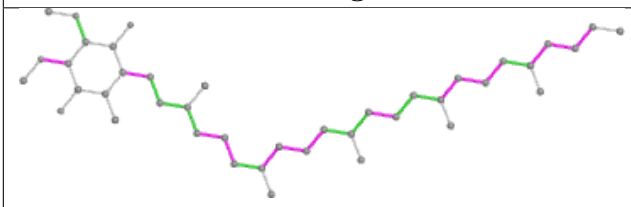
Ligand U10 L 285



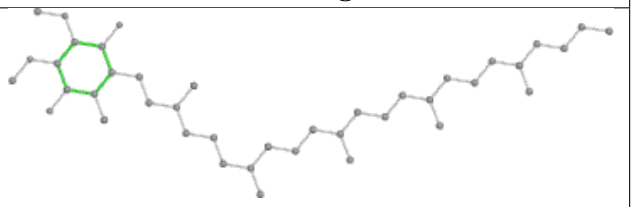
Bond lengths



Bond angles

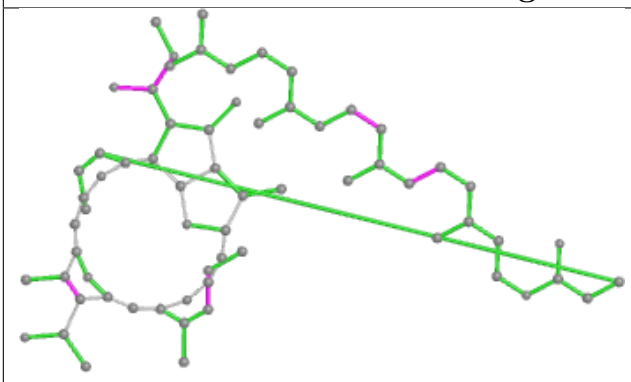


Torsions

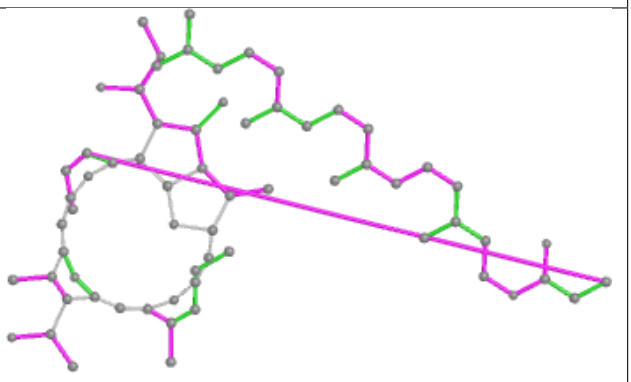


Rings

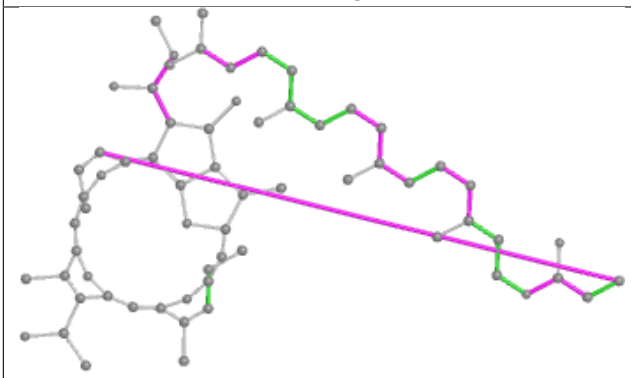
Ligand BPH M 312



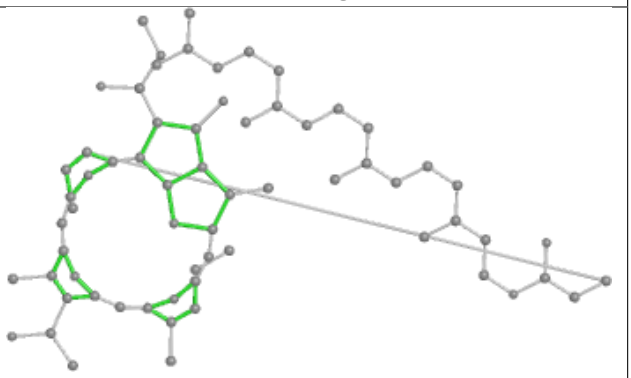
Bond lengths



Bond angles

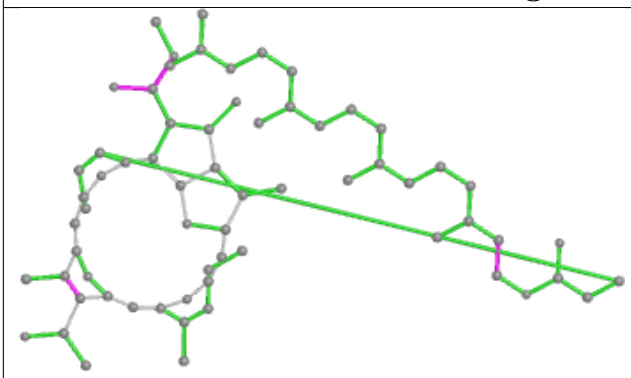


Torsions

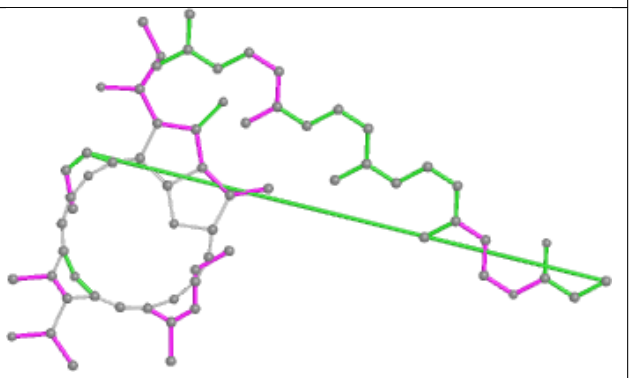


Rings

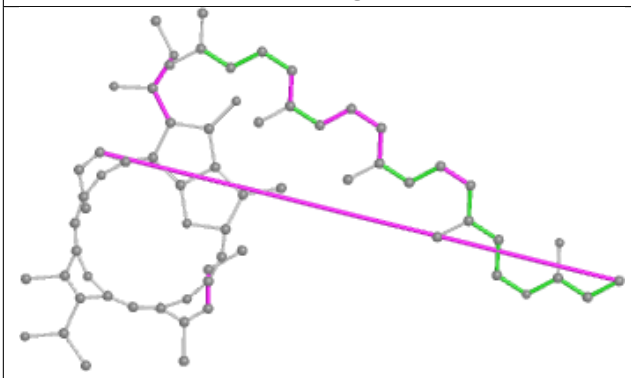
Ligand BPH L 284



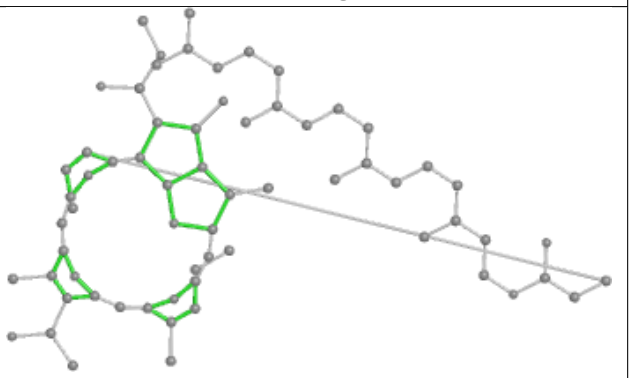
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	53:GLN	C	54:GLY	N	1.64
1	H	56:PHE	C	57:PRO	N	1.10

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.